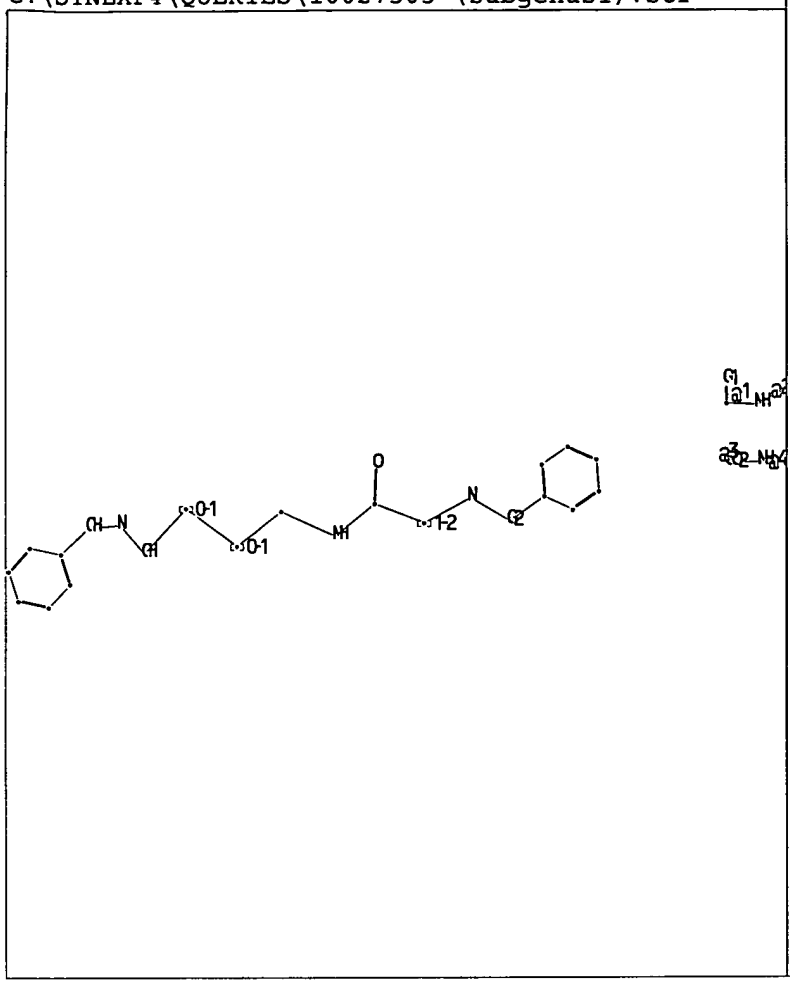
C:\STNEXP4\QUERIES\10027505 (subgenus1).str



X is $-CH-N-$

Z is present and is

$-SO_2-$;

O/S
$-C(=O)-NH-$

$\diamond-SO_2-NH-$

chain nodes :
2 3 4 5 6 8 9 15 16 19 20 21 22 23 24 40 41
ring nodes :
1 29 30 31 32 33 34 35 36 37 38 39
chain bonds :
1-2 2-3 3-15 4-5 4-8 6-9 15-16 16-19 16-20 20-21 21-22 22-23 23-24 24-41
29-40 40-41
ring bonds :
1-30 1-34 29-39 29-35 30-31 31-32 32-33 33-34 35-36 36-37 37-38 38-39
exact/norm bonds :
1-2 2-3 3-15 4-5 4-8 6-9 16-19 16-20 20-21 24-41 40-41
exact bonds :
15-16 21-22 22-23 23-24 29-40
normalized bonds :
1-30 1-34 29-39 29-35 30-31 31-32 32-33 33-34 35-36 36-37 37-38 38-39

G1:O,S

G2:SO2,[*1-*2],[*3-*4]

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 8:CLASS 9:CLASS 15:CLASS 16:CLASS
19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 29:Atom 30:CLASS 31:CLASS
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:CLASS 41:CLASS

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=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L1    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L2    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505 (subgenus1).str

L3      STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4   QUE L3 AND L1 NOT L2

=> d l4
L4 HAS NO ANSWERS
L1              SCR 1839
L2              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L3              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L4              QUE  L3 AND L1 NOT L2


=> s l4 sss sam
SAMPLE SEARCH INITIATED 10:50:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  37376 TO ITERATE

  2.7% PROCESSED    1000 ITERATIONS                              0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:       735992 TO   759048
PROJECTED ANSWERS:               0 TO        0

L5            0 SEA SSS SAM L3 AND L1 NOT L2

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L6    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
```

```
L7    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505 (subgenus1).str

L8      STRUCTURE UPLOADED

=> que L8 AND L6 NOT L7

L9   QUE L8 AND L6 NOT L7

=> d l9
L9 HAS NO ANSWERS
L6              SCR 1839
L7              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L8              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L9              QUE  L8 AND L6 NOT L7


=> s l9 sss sam
SAMPLE SEARCH INITIATED 10:51:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1022 TO ITERATE

 97.8% PROCESSED    1000 ITERATIONS                                2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        18523 TO    22357
PROJECTED ANSWERS:               2 TO      125

L10           2 SEA SSS SAM L8 AND L6 NOT L7

=> s l9 sss ful
FULL SEARCH INITIATED 10:51:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  20593 TO ITERATE

100.0% PROCESSED   20593 ITERATIONS                              54 ANSWERS
SEARCH TIME: 00.00.01

L11          54 SEA SSS FUL L8 AND L6 NOT L7

=> s l11
L12          7 L11

=> d l12 1-7 bib,ab,hitstr
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L12 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:412801 CAPLUS
DN 139:245782
TI Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease
IN Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy
PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SO PCT Int. Appl., 1243 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	WO 2003040096	A2	20030515	WO 2002-US36072	20021108
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2001-337122P	P	20011108		
	US 2001-344086P	P	20011228		
	US 2002-345635P	P	20020103		
	WO 2002-US36072	A	20021108		

OS MARPAT 139:245782
AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO2, (un)substituted NH; R4 = alkyl, haloalkyl, hydroxyalkyl, etc.; R5 = R6X (wherein X = CO, SO2, (un)substituted CH2; R6 = (un)substituted Ph, naphthyl, indanyl, etc.); R25 = H, alkyl, alkoxy, etc.] which have activity as inhibitors of .beta.-secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepd. E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC50 of < 20 .mu.M in cell free

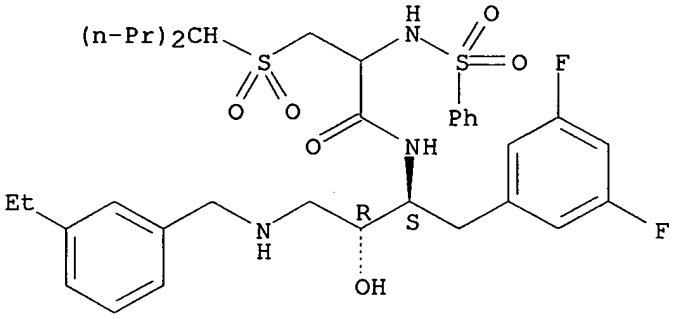
inhibition assay utilizing a synthetic APP substrate. This is a Part 2 of 1-2 series.

IT **477792-83-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

RN 477792-83-9 CAPLUS

CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]-2-[(phenylsulfonyl)amino]-3-[(1-propylbutyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:376819 CAPLUS
DN 138:385173
TI Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease
IN Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy
PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SO PCT Int. Appl., 1243 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003040096	A2	20030515	WO 2002-US36072	20021108
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2001-337122P	P	20011108		
	US 2001-344086P	P	20011228		
	US 2002-345635P	P	20020103		
	WO 2002-US36072	A	20021108		

OS MARPAT 138:385173
AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO2, (un)substituted NH; R4 = alkyl, haloalkyl, hydroxyalkyl, etc.; R5 = R6X (wherein X = CO, SO2, (un)substituted CH2; R6 = (un)substituted Ph, naphthyl, indanyl, etc.); R25 = H, alkyl, alkoxy, etc.] which have activity as inhibitors of .beta.-secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepd. E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC50 of < 20 .mu.M in cell free

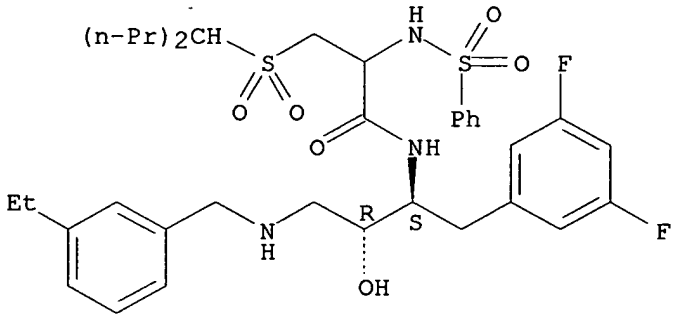
inhibition assay utilizing a synthetic APP substrate. This is a Part 1 of 1-2 series.

IT **477792-83-9P 527719-83-1P 527722-21-0P 527722-47-0P 527724-62-5P 527724-66-9P 527724-70-5P 527724-74-9P 527724-78-3P 527724-81-8P 527724-86-3P 527725-01-5P 527725-60-6P 527726-09-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

RN 477792-83-9 CAPLUS

CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]-2-[(phenylsulfonyl)amino]-3-[(1-propylbutyl)sulfonyl]- (9CI) (CA INDEX NAME)

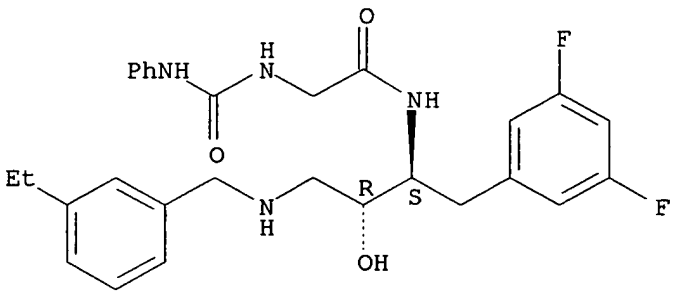
Absolute stereochemistry.



RN 527719-83-1 CAPLUS

CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]-2-[[(phenylamino)carbonyl]amino]- (9CI) (CA INDEX NAME)

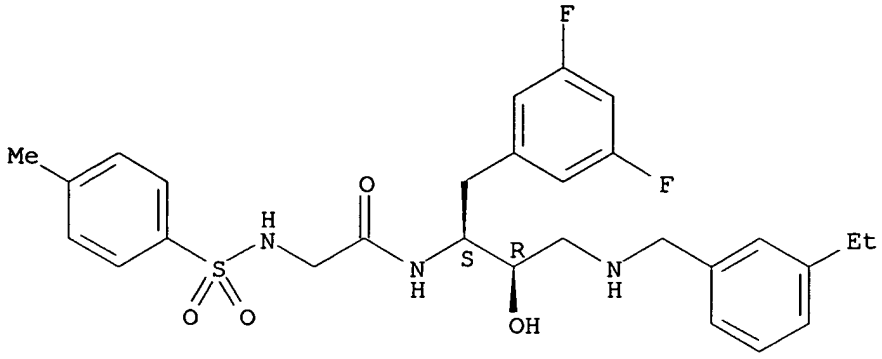
Absolute stereochemistry.



RN 527722-21-0 CAPLUS

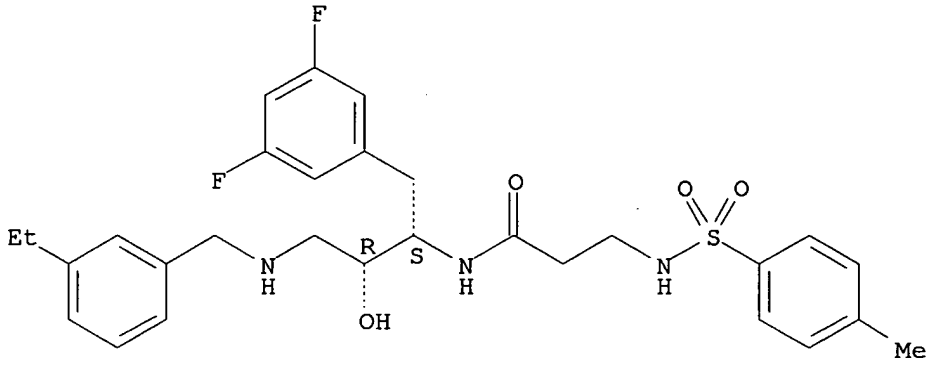
CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]-2-[[(4-methylphenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



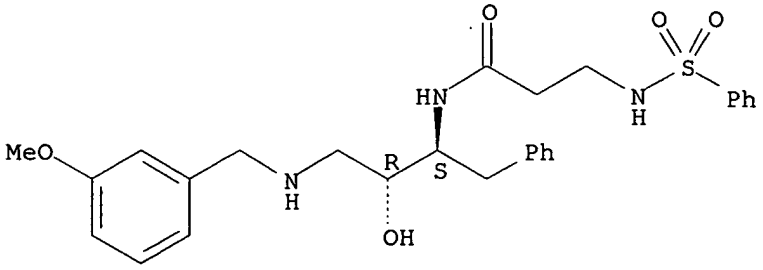
RN 527722-47-0 CAPLUS
CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]-3-[[(4-methylphenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



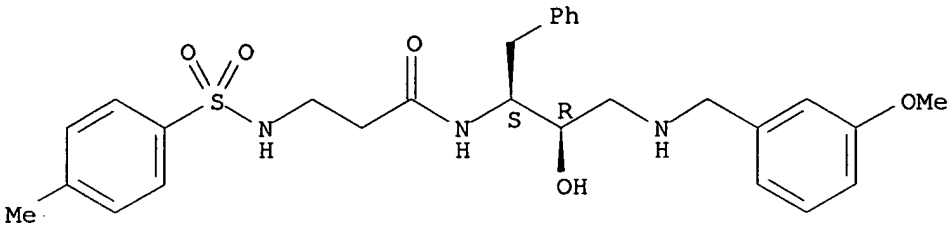
RN 527724-62-5 CAPLUS
CN Propanamide, N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-3-[(phenylsulfonyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



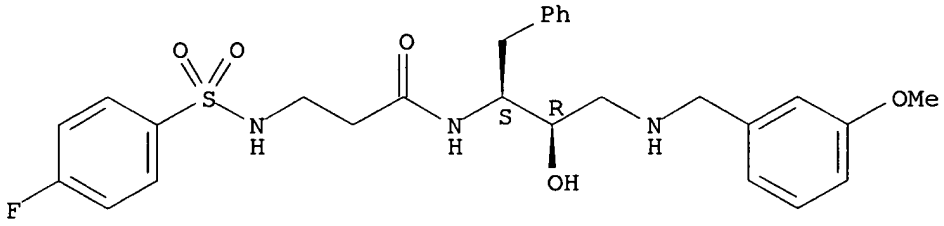
RN 527724-66-9 CAPLUS
CN Propanamide, N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-3-[[(4-methylphenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



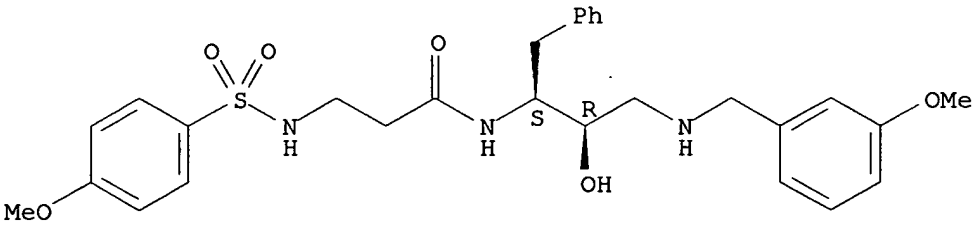
RN 527724-70-5 CAPLUS
CN Propanamide, 3-[[(4-fluorophenyl)sulfonyl]amino]-N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



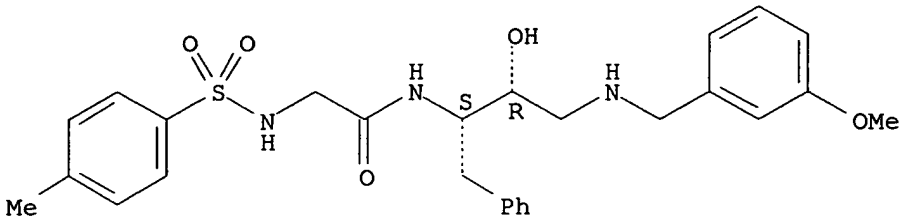
RN 527724-74-9 CAPLUS
CN Propanamide, N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-3-[[(4-methoxyphenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



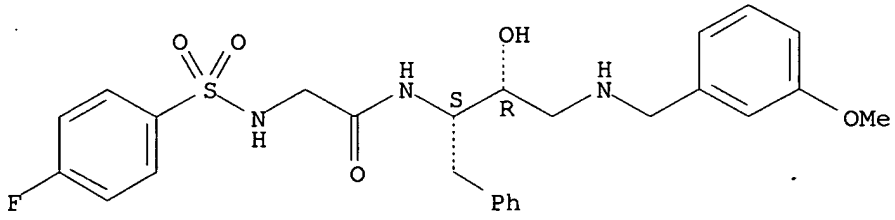
RN 527724-78-3 CAPLUS
CN Acetamide, N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-2-[[(4-methylphenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



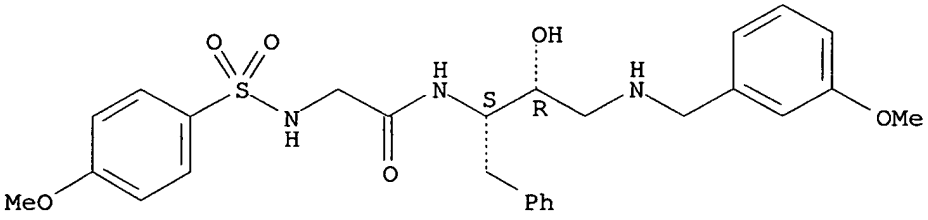
RN 527724-81-8 CAPLUS
CN Acetamide, 2-[[(4-fluorophenyl)sulfonyl]amino]-N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



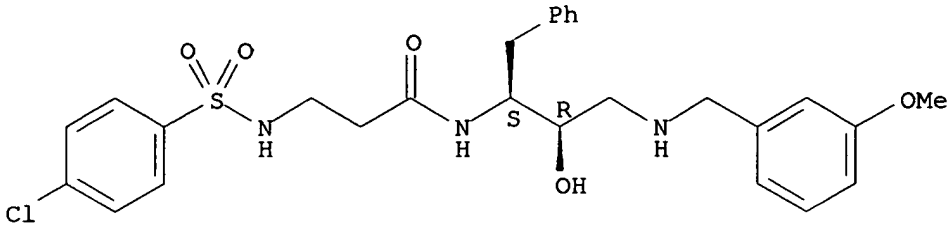
RN 527724-86-3 CAPLUS
CN Acetamide, N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-2-[[(4-methoxyphenyl)sulfonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



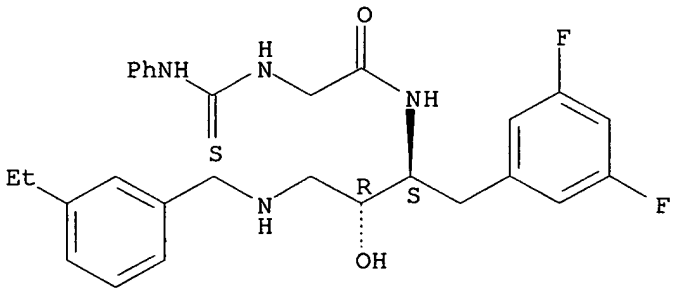
RN 527725-01-5 CAPLUS
CN Propanamide, 3-[[(4-chlorophenyl)sulfonyl]amino]-N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



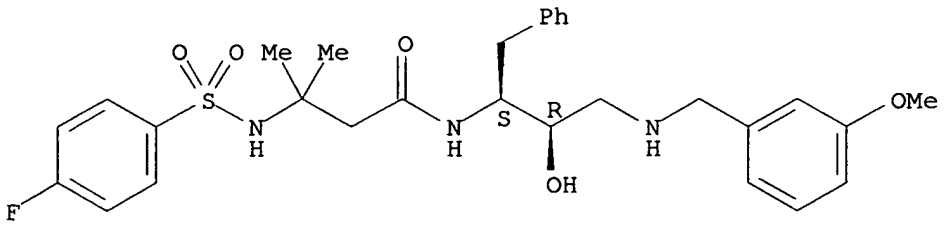
RN 527725-60-6 CAPLUS
CN Acetamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]-2-[[(phenylamino)thioxomethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 527726-09-6 CAPLUS
CN Butanamide, 3-[[(4-fluorophenyl)sulfonyl]amino]-N-[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

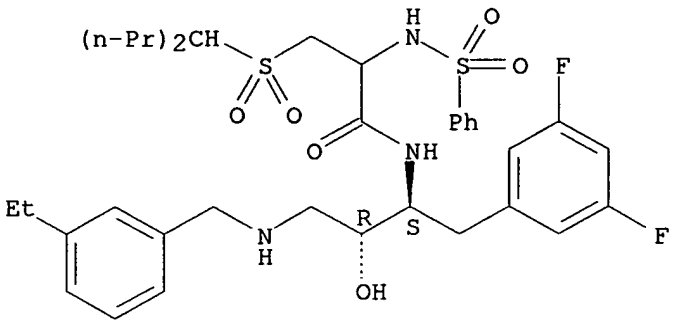


L12 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:946261 CAPLUS
DN 138:14180
TI Preparation of peptide-related hydroxyalkylamines for pharmaceutical use in the treatment of Alzheimer's disease
IN Freskos, John; Aquino, Jose; Brown, David L.; Fang, Larry; Fobian, Yvette M.; Gailunas, Andrea; Guinn, Ashley; Varghese, John; Romero, Arthur Glenn; Tucker, John; Tung, Jay; Walker, Donald
PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SO PCT Int. Appl., 360 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002098849	A2	20021212	WO 2002-US17698	20020531
	WO 2002098849	A3	20031113		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2003166717	A1	20030904	US 2002-160777	20020531
PRAI	US 2001-295332P	P	20010601		
	US 2001-332639P	P	20011119		
	US 2001-343772P	P	20011228		

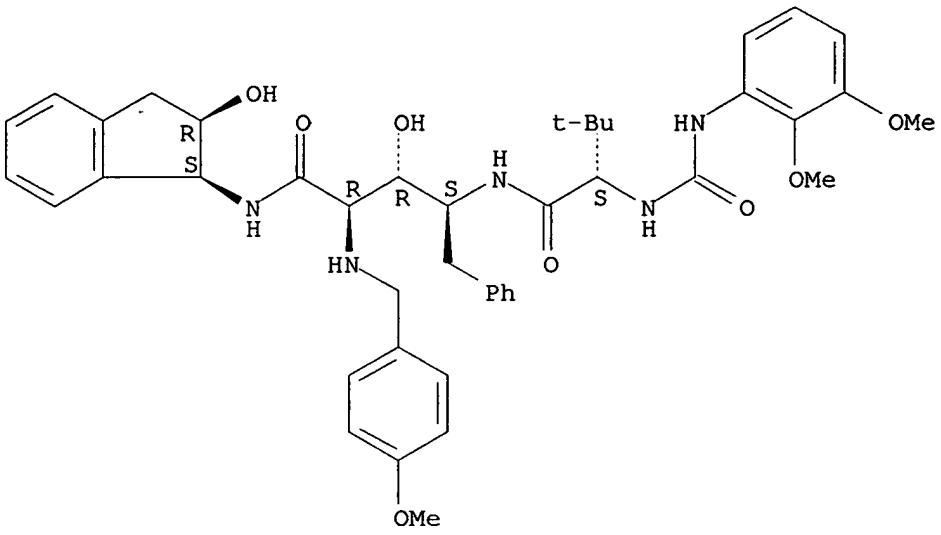
OS MARPAT 138:14180
AB Hydroxyalkylamines RNNR20CHR1CH(OH)CR2R3NR20Rc [RN is an acyl group of defined structure; R20 is H, (un)substituted alkyl, alkoxy, alkoxy-, hydroxy-, or haloalkyl, or -R26-R27, where R26 is CO, SO2, CO2, CONH, or alkylcarbamoyl and R27 is (un)substituted alkyl, alkoxy, arylalkyl, heterocycloalkyl, or heteroaryl; R1 is -(CH2)1-2-S(O)0-2-alkyl, (un)substituted alkyl, alkenyl, alkynyl, (hetero)aryl, heterocyclyl, etc.; R2, R3 are H or (un)substituted alkyl or CR2R3 is a 3-7 membered carbocycle in which one carbon atom is optionally replaced by O, S, SO2, or NRN-2; Rc is (un)substituted alkyl, (hetero)arylalkyl, heterocyclylalkyl, etc.] were prepd. for treating Alzheimer's disease and similar diseases. Synthetic procedures are given in examples and schemes. Several hundred products of the invention are listed in a table and in the claims, including S-butyl-N-1-[(1S,2R)-1-(3,5-difluorobenzyl)-3-[(3-ethylbenzyl)amino]-2-hydroxypropyl]-D-cysteinamide.
IT **477792-83-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of peptide-related hydroxyalkylamines for treatment of Alzheimer's disease)
RN 477792-83-9 CAPLUS
CN Propanamide, N-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]-2-[(phenylsulfonyl)amino]-3-[(1-propylbutyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:241976 CAPLUS
DN 124:331828
TI Inhibitors of Human Immunodeficiency Virus Type 1 Protease Containing 2-Aminobenzyl-Substituted 4-Amino-3-hydroxy-5-phenylpentanoic acid: Synthesis, Activity, and Oral Bioavailability
AU Lehr, Philipp; Billich, Andreas; Charpiot, Brigitte; Ettmayer, Peter; Scholz, Dieter; Rosenwirth, Brigitte; Gstach, Hubert
CS Sandoz Research Institute, Vienna, A-1235, Austria
SO Journal of Medicinal Chemistry (1996), 39(10), 2060-7
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB Systematic modifications of HIV protease inhibitor (2R,3S,4S)-4-[[(benzyloxycarbonyl)-L-valyl]amino]-3-hydroxy-2-[(4-methoxybenzyl)amino]-5-(phenylpentanoyl)-L-valine 2-(aminomethyl)benzimidazole amide led to a novel series of inhibitors with a shortened, modified carboxy terminus. Their synthesis, in vitro enzyme inhibitory data, and antiviral activities are reported. Of particular interest are derivs. featuring the (1S,2R)-1-amino-2-hydroxyindan moiety at the P2'-position since some of them exhibit substantial oral bioavailability in mice. The influence of aq. soly. and structural parameters on the oral resorption of the inhibitors is discussed. Optimum enhancement of oral bioavailability was obsd. with L-tert-leucine in P2-position, resulting in the discovery of (2R,3S,4S)-4-[[(benzyloxycarbonyl)-L-tert-leucyl]amino]-3-hydroxy-2-[(4-methoxybenzyl)amino]-5-phenylpentanoic acid (1S,2R)-1-amino-2-hydroxyindan amide which combines high antiviral activity (IC50 = 250 nM) with a good pharmacokinetic profile (AUC = 82.5 .mu.M.cntdot.h at a dose of 125 mg/kg po in mice).
IT **176389-02-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and bioavailability and HIV-1 protease inhibitory activity of (aminobenzyl)hydroxyphenylpentanoates)
RN 176389-02-9 CAPLUS
CN L-Lyxonamide, 2,4,5-trideoxy-N-(2,3-dihydro-2-hydroxy-1H-inden-1-yl)-4-[[2-[[[(2,3-dimethoxyphenyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]amino]-2-[[(4-methoxyphenyl)methyl]amino]-5-phenyl-, [1(1S,2R),4(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


OH
R
S
O
OH
t-Bu
HN
OMe
H
N
R
R
S
S
N
H
N
H
O
OMe
HN
Ph
OMe

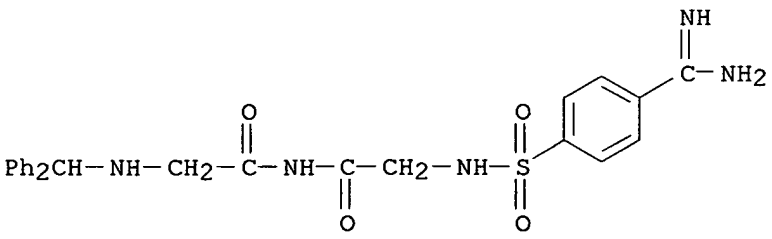
L12 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1995:820544 CAPLUS
DN 123:227821
TI Preparation of 4-amidinophenylsulfonamide antithrombotics
IN Leinert, Herbert; Poll, Thomas; von der Saal, Wolfgang; Stegmeier, Karlheinz
PA Boehringer Mannheim G.m.b.H., Germany
SO Ger. Offen., 10 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4316922	A1	19941124	DE 1993-4316922	19930520
	WO 9427958	A1	19941208	WO 1994-EP1562	19940513
	W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, KZ, NO, NZ, PL, RO, RU, SI, SK, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9469278	A1	19941220	AU 1994-69278	19940513
PRAI	DE 1993-4316922		19930520		
	WO 1994-EP1562		19940513		

OS MARPAT 123:227821
AB The title compds. (I; A = .alpha.-amino acid residue; B = H, A; R1, R2 = H, Ph, CO2H, alkoxycarbonyl), useful as agents for treating thromboembolic diseases (no data), are prepd.
IT **168258-23-9P 168258-25-1P 168258-31-9P**
168258-33-1P 168258-35-3P 168258-37-5P
168258-39-7P 168258-41-1P 168258-43-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 4-amidinophenylsulfonamide antithrombotics)
RN 168258-23-9 CAPLUS
CN Acetamide, N-[[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]acetyl]-2-[(diphenylmethyl)amino]-, monoacetate (9CI) (CA INDEX NAME)

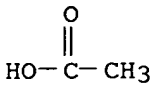
CM 1

CRN 168258-22-8
CMF C24 H25 N5 O4 S



CM 2

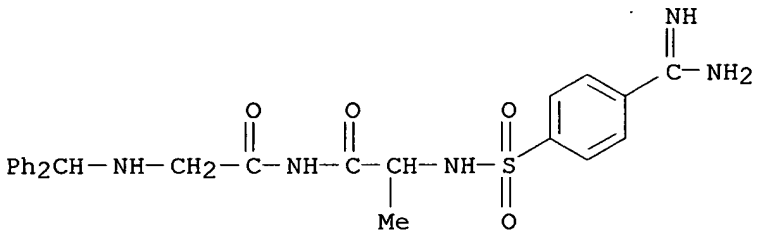
CRN 64-19-7
CMF C2 H4 O2



RN 168258-25-1 CAPLUS
CN Propanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-, monoacetate (9CI) (CA INDEX NAME)

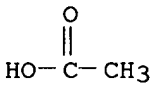
CM 1

CRN 168258-24-0
CMF C25 H27 N5 O4 S



CM 2

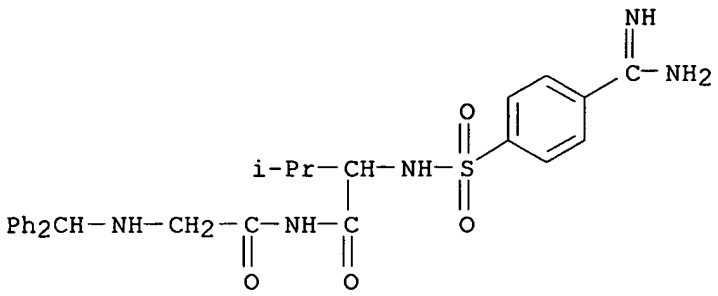
CRN 64-19-7
CMF C2 H4 O2



RN 168258-31-9 CAPLUS
CN Butanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-3-methyl-, monoacetate (9CI) (CA INDEX NAME)

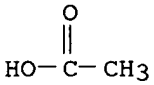
CM 1

CRN 168258-30-8
CMF C27 H31 N5 O4 S



CM 2

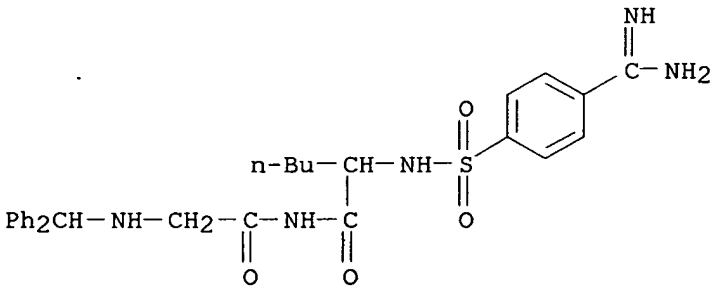
CRN 64-19-7
CMF C2 H4 O2



RN 168258-33-1 CAPLUS
CN Hexanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-, monoacetate (9CI) (CA INDEX NAME)

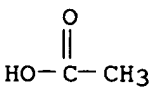
CM 1

CRN 168258-32-0
CMF C28 H33 N5 O4 S



CM 2

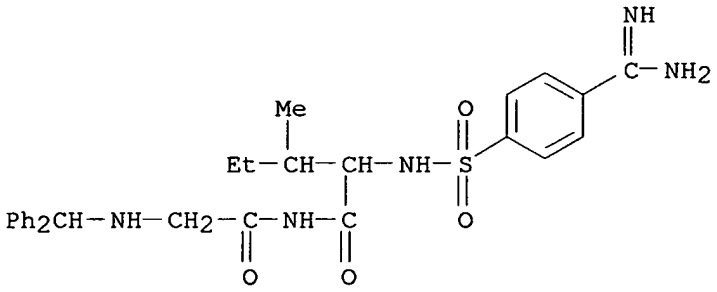
CRN 64-19-7
CMF C2 H4 O2



RN 168258-35-3 CAPLUS
CN Pentanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-3-methyl-, monoacetate (9CI) (CA INDEX NAME)

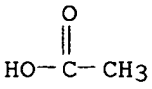
CM 1

CRN 168258-34-2
CMF C28 H33 N5 O4 S



CM 2

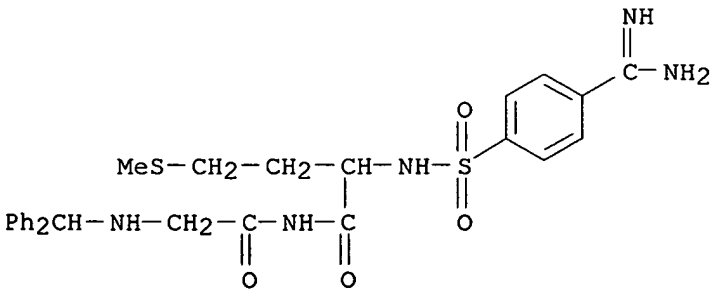
CRN 64-19-7
CMF C2 H4 O2



RN 168258-37-5 CAPLUS
CN Butanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-(methylthio)-, monoacetate (9CI) (CA INDEX NAME)

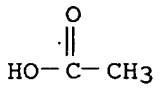
CM 1

CRN 168258-36-4
CMF C27 H31 N5 O4 S2



CM 2

CRN 64-19-7
CMF C2 H4 O2

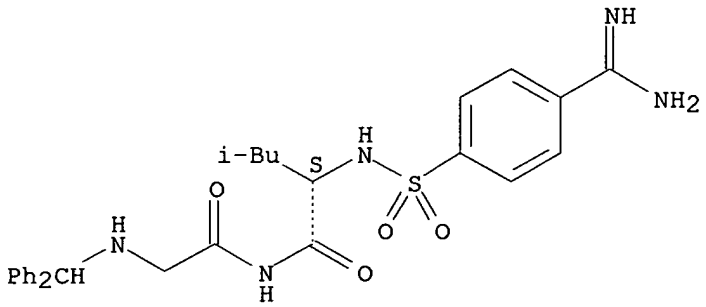


RN 168258-39-7 CAPLUS
CN Pentanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-methyl-, (S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

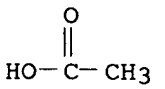
CRN 168258-38-6
CMF C28 H33 N5 O4 S

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2



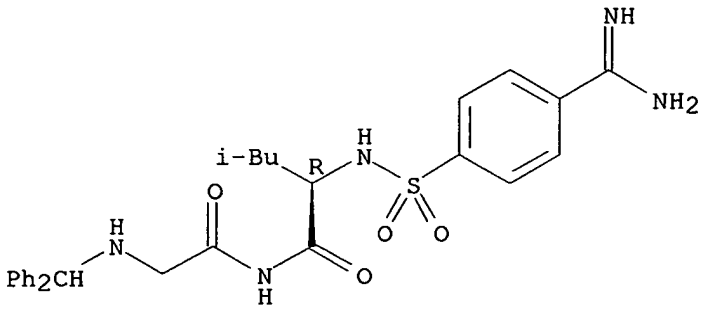
RN 168258-41-1 CAPLUS
CN Pentanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-methyl-, (R)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 168258-40-0

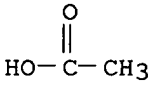
CMF C28 H33 N5 O4 S

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2

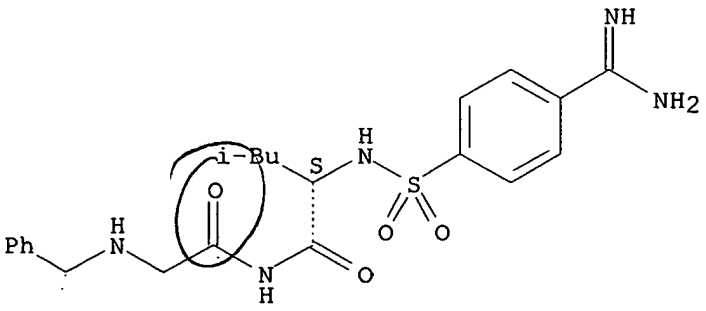


RN 168258-43-3 CAPLUS
CN Pentanamide, 2-[[[4-(aminoiminomethyl)phenyl]sulfonyl]amino]-4-methyl-N-[[(phenylmethyl)amino]acetyl]-, (S)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

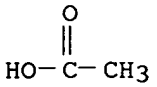
CRN 168258-42-2
CMF C22 H29 N5 O4 S

Absolute stereochemistry.



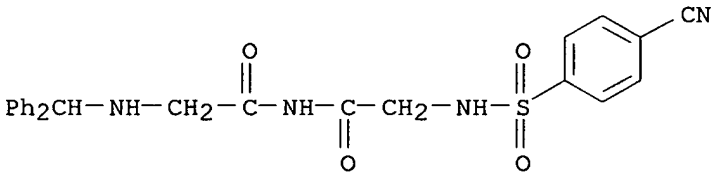
CM 2

CRN 64-19-7
CMF C2 H4 O2

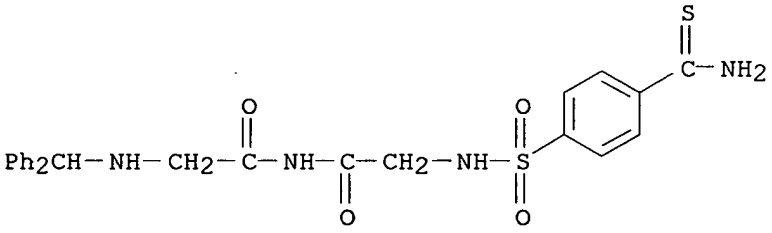


IT **168258-49-9P 168258-50-2P 168258-53-5P**
168258-54-6P 168258-63-7P 168258-64-8P
168258-67-1P 168258-68-2P 168258-71-7P
168258-72-8P 168258-74-0P 168258-75-1P
168258-78-4P 168258-79-5P 168258-82-0P
168258-83-1P 168258-86-4P 168258-87-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 4-amidinophenylsulfonamide antithrombotics from)

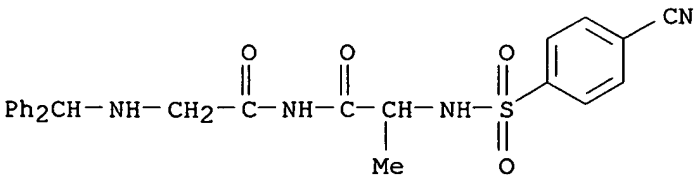
RN 168258-49-9 CAPLUS
CN Acetamide, N-[[[(4-cyanophenyl)sulfonyl]amino]acetyl]-2-[(diphenylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 168258-50-2 CAPLUS
CN Acetamide, N-[[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]acetyl]-2-[(diphenylmethyl)amino]- (9CI) (CA INDEX NAME)

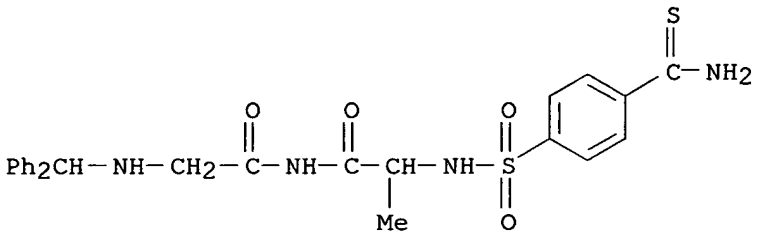


RN 168258-53-5 CAPLUS
CN Propanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]- (9CI) (CA INDEX NAME)

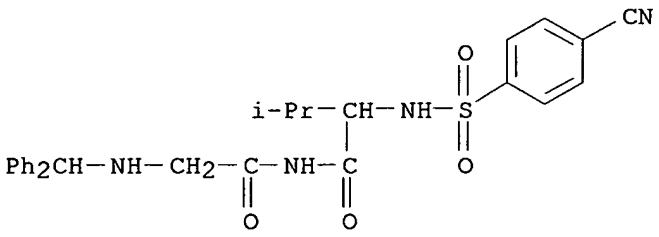


RN 168258-54-6 CAPLUS

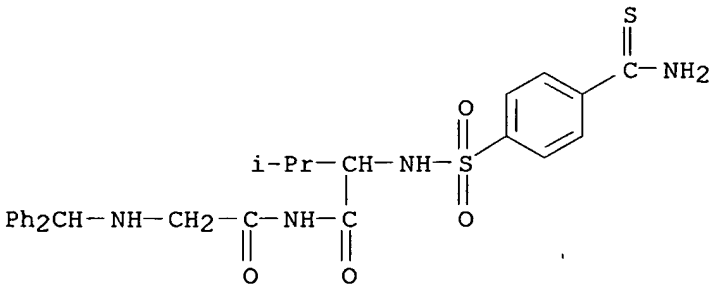
CN Propanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]- (9CI) (CA INDEX NAME)



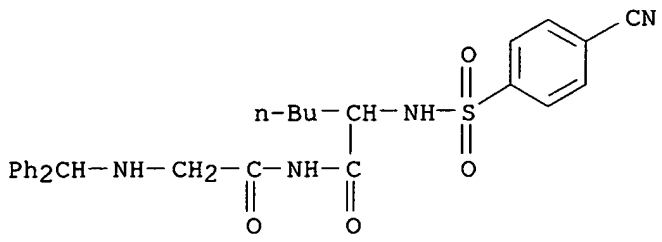
RN 168258-63-7 CAPLUS
CN Butanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-3-methyl- (9CI) (CA INDEX NAME)



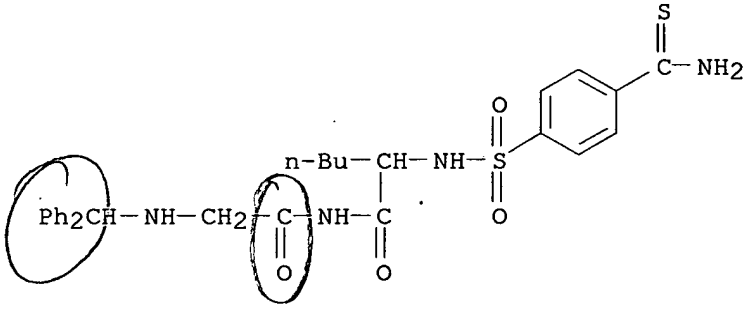
RN 168258-64-8 CAPLUS
CN Butanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-3-methyl- (9CI) (CA INDEX NAME)



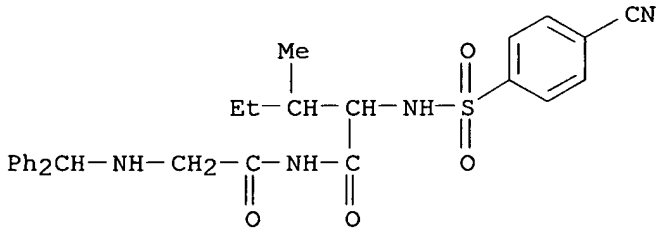
RN 168258-67-1 CAPLUS
CN Hexanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]- (9CI) (CA INDEX NAME)



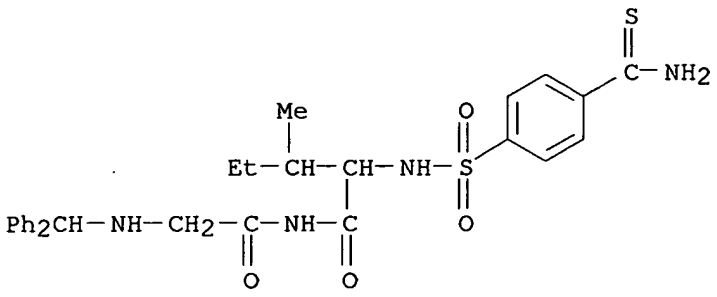
RN 168258-68-2 CAPLUS
CN Hexanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]- (9CI) (CA INDEX NAME)



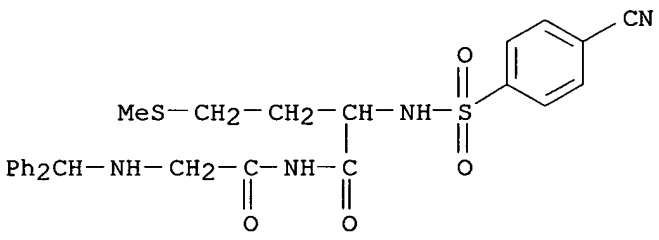
RN 168258-71-7 CAPLUS
CN Pentanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-3-methyl- (9CI) (CA INDEX NAME)



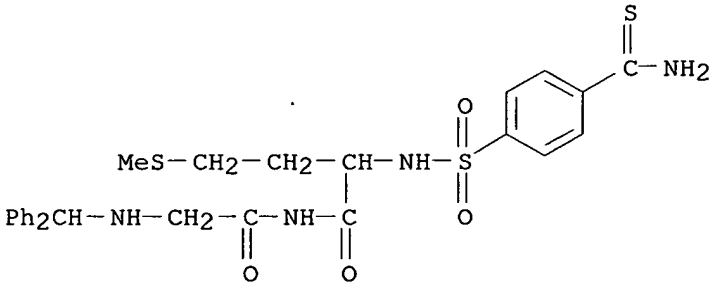
RN 168258-72-8 CAPLUS
CN Pentanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-3-methyl- (9CI) (CA INDEX NAME)



RN 168258-74-0 CAPLUS
CN Butanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-(methylthio)- (9CI) (CA INDEX NAME)

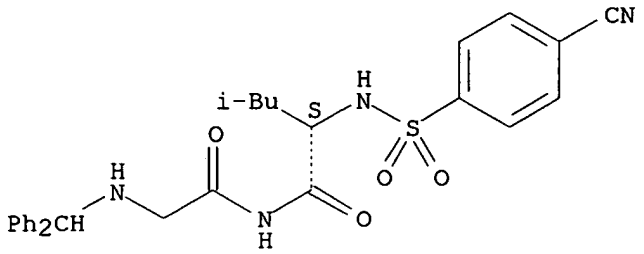


RN 168258-75-1 CAPLUS
CN Butanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-(methylthio)- (9CI) (CA INDEX NAME)



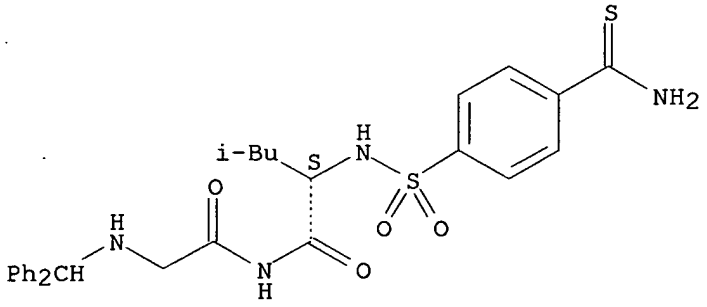
RN 168258-78-4 CAPLUS
CN Pentanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-methyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



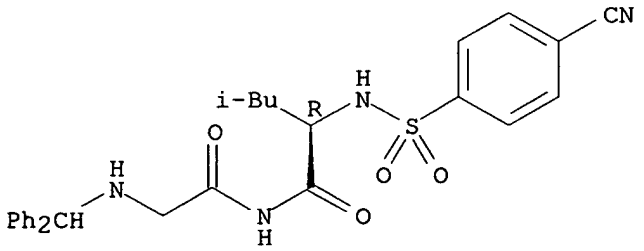
RN 168258-79-5 CAPLUS
CN Pentanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-methyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



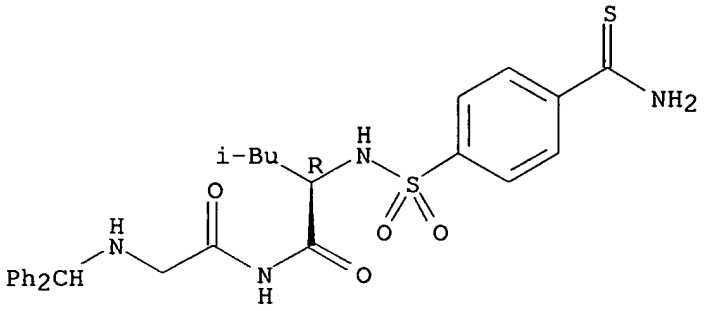
RN 168258-82-0 CAPLUS
CN Pentanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-methyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



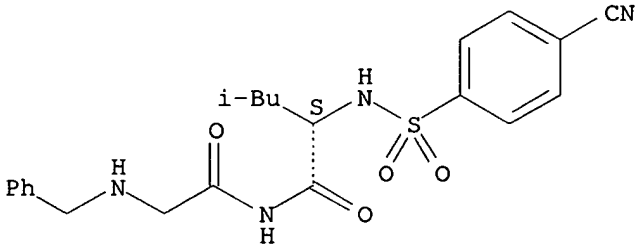
RN 168258-83-1 CAPLUS
CN Pentanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-N-[[(diphenylmethyl)amino]acetyl]-4-methyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



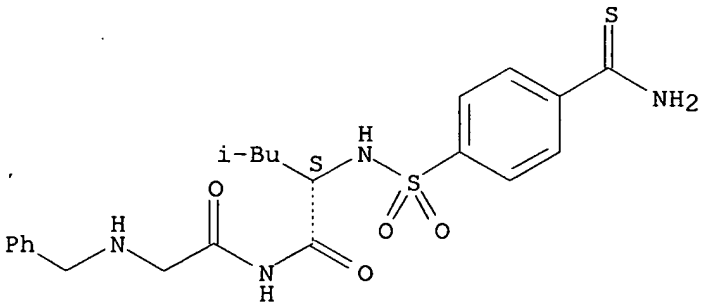
RN 168258-86-4 CAPLUS
CN Pentanamide, 2-[[(4-cyanophenyl)sulfonyl]amino]-4-methyl-N-[[(phenylmethyl)amino]acetyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 168258-87-5 CAPLUS
CN Pentanamide, 2-[[[4-(aminothioxomethyl)phenyl]sulfonyl]amino]-4-methyl-N-[[(phenylmethyl)amino]acetyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

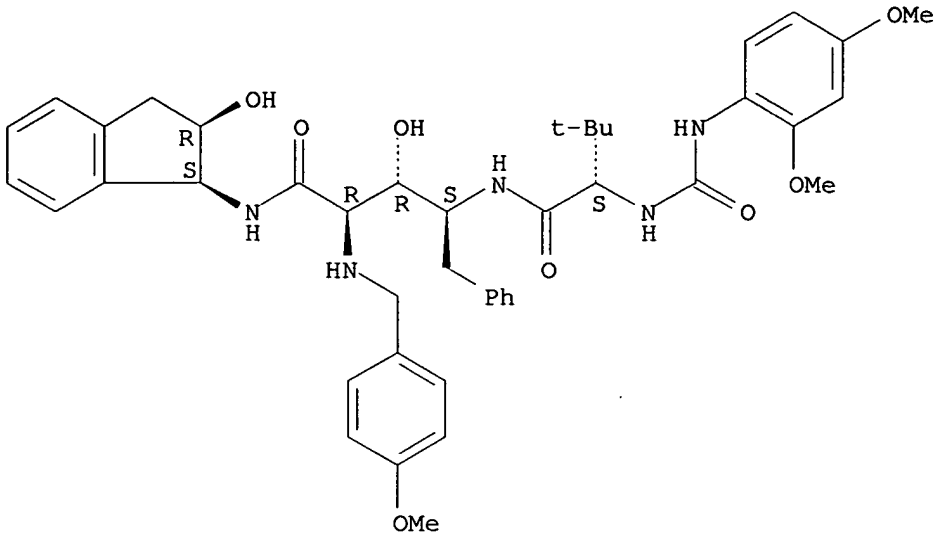


L12 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1995:657540 CAPLUS
DN 123:82953
TI Preparation of 2,4-diamino-3-hydroxycarboxylic acid-derivative HIV proteinase inhibitors.
IN Billich, Andreas; Charpiot, Brigitte; Ettmayer, Peter; Gstach, Hubert; Lehr, Philipp; Scholz, Dieter
PA Sandoz Ltd., Switz.; Sandoz-Patent-G.m.b.H.; Sandoz-Erfindungen Verwaltungsgesellschaft m.b.H.
SO Eur. Pat. Appl., 19 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 615969	A1	19940921	EP 1994-810150	19940309
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	US 5538997	A	19960723	US 1994-177687	19940103
	NO 9400844	A	19940913	NO 1994-844	19940310
	AU 9457737	A1	19940915	AU 1994-57737	19940310
	AU 672867	B2	19961017		
	FI 9401149	A	19941222	FI 1994-1149	19940310
	CA 2118876	AA	19940913	CA 1994-2118876	19940311
	JP 07089919	A2	19950404	JP 1994-41047	19940311
	CN 1104209	A	19950628	CN 1994-102292	19940311
	ZA 9401734	A	19950911	ZA 1994-1734	19940311
	HU 71793	A2	19960228	HU 1994-745	19940311
PRAI	GB 1993-5144		19930312		
	GB 1993-19667		19930923		

OS MARPAT 123:82953
AB The title compds. [I; A, B = direct bond (un)substituted aminoacyl moiety; R1 = H, amino-protecting group, etc.; R2 = side chain of a natural amino acid, (un)substituted alkyl, cycloalkyl, etc; R3 = halogen, alkyl, alkoxy, hydroxyalkoxy; R4 = 2(R)-hydroxyindan-1(S)-yl, (un)substituted 2-hydroxybenzyl, (S)-2-hydroxy-1-phenylethyl], useful as inhibitors of HIV proteinase (no data) for the treatment of HIV-induced diseases (e.g., AIDS) (no data), are prepd. Thus, 4(S)-tert-butoxycarbonylamino-3(S)-hydroxy-2(R)-(4-methoxybenzylamino)-5-phenylpentanoic acid 1(S)-amino-2(R)-hydroxyindan-amide, m.p. 183-185.degree., was prepd. from BOC-L-alaninol in 5 steps.
IT **164514-82-3P 164515-00-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 2,4-diamino-3-hydroxycarboxylic acid-deriv. HIV proteinase inhibitors)
RN 164514-82-3 CAPLUS
CN Benzenepentanamide, N-(2,3-dihydro-2-hydroxy-1H-inden-1-yl)-.gamma.-[[2-[[[(2,4-dimethoxyphenyl)amino]carbonyl]amino]-3,3-dimethyl-1-oxobutyl]amino]-.beta.-hydroxy-.alpha.-[[(4-methoxyphenyl)methyl]amino]-, [1S-[1.alpha.[.alpha.S*,.beta.S*,.gamma.R*(R*)],2.alpha.]]- (9CI) (CA INDEX NAME)

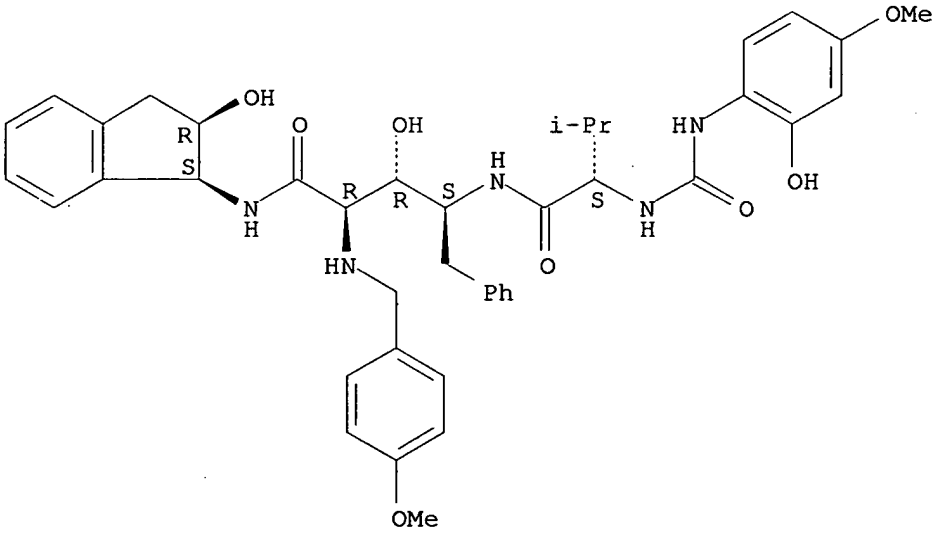
Absolute stereochemistry.



RN 164515-00-8 CAPLUS

CN Benzenepentanamide, N-(2,3-dihydro-2-hydroxy-1H-inden-1-yl)-.beta.-hydroxy-.gamma.-[[2-[[[(2-hydroxy-4-methoxyphenyl)amino]carbonyl]amino]-3-methyl-1-oxobutyl]amino]-.alpha.-[[(4-methoxyphenyl)methyl]amino]-, [1S-[1.alpha.[.alpha.S*,.beta.S*,.gamma.R*(R*)],2.alpha.]]- (9CI) (CA INDEX NAME)

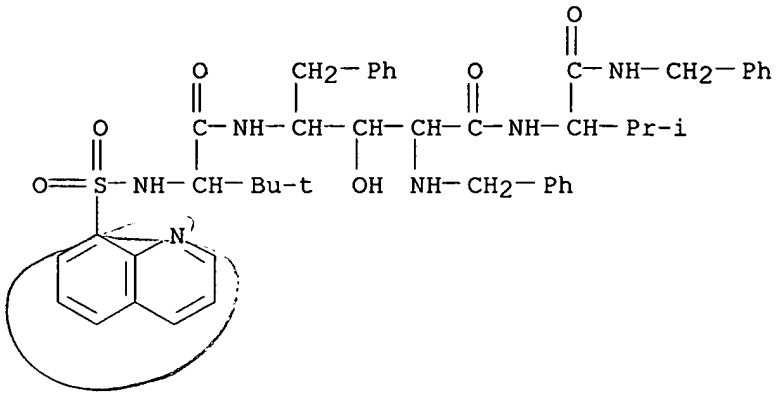
Absolute stereochemistry.



L12 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1993:473121 CAPLUS
DN 119:73121
TI 4-amino-3-hydroxycarboxylic acid derivatives
IN Billich, Andreas; Charpiot, Brigitte; Lehr, Philip; Scholz, Dieter
PA Sandoz Ltd., Switz.; Sandoz-Patent-G.m.b.H.
SO PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

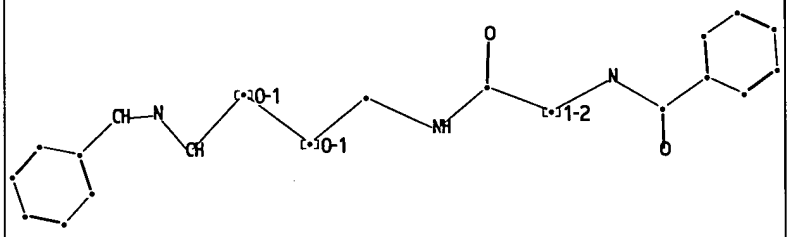
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9301166	A1	19930121	WO 1992-EP1471	19920630
	W: AU, CA, CS, FI, HU, JP, KR, NO, PL, RO, RU, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
	CA 2109326	AA	19930103	CA 1992-2109326	19920630
	AU 9221944	A1	19930211	AU 1992-21944	19920630
	EP 594656	A1	19940504	EP 1992-913821	19920630
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 07501786	T2	19950223	JP 1992-501937	19920630
	ZA 9204932	A	19940103	ZA 1992-4932	19920702
	CN 1088912	A	19940706	CN 1993-100562	19930101
PRAI	GB 1991-14261		19910702		
	GB 1991-23721		19911107		
	GB 1992-3884		19920224		
	WO 1992-EP1471		19920630		

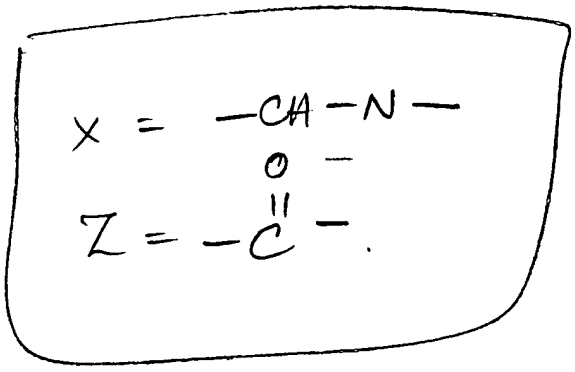
OS MARPAT 119:73121
AB Title compds. I [A and B = bond or (un)substituted amino acid residue; R1 = H, amino protecting group, R6Y (R6 = H, alkyl, alkenyl, alkynyl, aryl, aralkyl, heteroaryl, etc.; Y = CO, NHCO,NHCS, SO2, OCO, OCS); R2 = amino acid side chain, alkyl, aralkyl, trimethylsilylmethyl, 2-thienylmethyl, etc.; R3 = alkyl, alkenyl, alkynyl, cycloalkyl, aryl, etc.; R4 = OR7 or NHR7 where R7 has the meaning indicated for R6; X = S or NR5 (R5 = H, Me, HCO, Ac) were prepd. antiviral agents, particularly HIV-1 proteinase inhibitors. Thus, Z-L-Val-OC6H4NO2-p (Z = PhCH2O2C) was coupled with L-phenylalaninol (Phe-ol) in the presence of Et3N in DMF to give Z-L-Val-L-Phe-ol, which underwent the Swern oxidn. with oxalyl chloride and DMSO to give the aldehyde, which underwent the Wittig reaction with Ph3P:CHCO2Et in toluene to give alkene II, which underwent epoxidn. with m-chloroperbenzoic acid in CH2Cl2 to give epoxide III. The epoxide of III was cleaved by PhCH2NH2 to give title compd. IV. I were measured for their ability to inhibit HIV proteinase and to inhibit the cellular HIV-induced cytopathic effect.
IT **148742-80-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as HIV proteinase inhibitor)
RN 148742-80-7 CAPLUS
CN Pentonamide, 2,4,5-trideoxy-4-[[3,3-dimethyl-1-oxo-2-[(8-quinolinylsulfonyl)amino]butyl]amino]-N-[2-methyl-1-[[(phenylmethyl)amino]carbonyl]propyl]-5-phenyl-2-[(phenylmethyl)amino]-, [1(S),4(S)]- (9CI) (CA INDEX NAME)



```
=> d his

     (FILE 'HOME' ENTERED AT 10:50:08 ON 29 DEC 2003)

     FILE 'REGISTRY' ENTERED AT 10:50:14 ON 29 DEC 2003
L1             SCREEN 1839
L2             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L3             STRUCTURE UPLOADED
L4             QUE L3 AND L1 NOT L2
L5           0 S L4 SSS SAM
L6             SCREEN 1839
L7             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L8             STRUCTURE UPLOADED
L9             QUE L8 AND L6 NOT L7
L10          2 S L9 SSS SAM
L11         54 S L9 SSS FUL

     FILE 'CAPLUS' ENTERED AT 10:51:53 ON 29 DEC 2003
L12          7 S L11

     FILE 'CAOLD' ENTERED AT 10:54:00 ON 29 DEC 2003

=> s l11
L13          0 L11

=> log y
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.40     182.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -4.56

STN INTERNATIONAL LOGOFF AT 10:54:12 ON 29 DEC 2003
```

C:\STNEXP4\QUERIES\10027505 (examples).str





No Cyclic moieties in Chain.

chain nodes :
2 3 4 7 8 9 10 11 12 28 29 30 31
ring nodes :
1 17 18 19 20 21 22 23 24 25 26 27
chain bonds :
1-30 2-3 2-30 3-4 4-7 4-8 8-9 9-10 10-11 11-12 12-29 17-28 28-29 30-31
ring bonds :
1-22 1-18 17-27 17-23 18-19 19-20 20-21 21-22 23-24 24-25 25-26 26-27
exact/norm bonds :
2-3 2-30 4-7 4-8 8-9 12-29 28-29 30-31
exact bonds :
1-30 3-4 9-10 10-11 11-12 17-28
normalized bonds :
1-22 1-18 17-27 17-23 18-19 19-20 20-21 21-22 23-24 24-25 25-26 26-27

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS
17:Atom 18:CLASS 19:CLASS 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom
27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS

```
=>
Uploading 10027505 (amended).str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 10:20:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  88268 TO ITERATE

  1.1% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS       0

L2            0 SEA SSS SAM L1

=>
Uploading 10027505 (amended).str

L3      STRUCTURE UPLOADED

=> d l3
L3 HAS NO ANSWERS
L3              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l3 sss sam
SAMPLE SEARCH INITIATED 10:23:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  27481 TO ITERATE

  3.6% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      539719 TO   559521
PROJECTED ANSWERS:              0 TO        0

L4            0 SEA SSS SAM L3
```

```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L5    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L6    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505 (amended).str

L7      STRUCTURE UPLOADED

=> que L7 AND L5 NOT L6

L8   QUE L7 AND L5 NOT L6

=> d 18
L8 HAS NO ANSWERS
L5              SCR 1839
L6              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L7              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L8              QUE  L7 AND L5 NOT L6


=> s l8 sss sam
SAMPLE SEARCH INITIATED 10:25:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  25710 TO ITERATE

  3.9% PROCESSED    1000 ITERATIONS                              1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       504621 TO   523779
PROJECTED ANSWERS:             210 TO      818

L9            1 SEA SSS SAM L7 AND L5 NOT L6

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839 AND 1994

L10   SCREEN CREATED
```

```
=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L11   SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505 (amended).str

L12     STRUCTURE UPLOADED

=> que L12 AND L10 NOT L11

L13  QUE L12 AND L10 NOT L11

=> d l13
L13 HAS NO ANSWERS
L10             SCR 1839 AND 1994
L11             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L12             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L13             QUE  L12 AND L10 NOT L11


=> s l13 sss sam
SAMPLE SEARCH INITIATED 10:27:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  37376 TO ITERATE

  2.7% PROCESSED    1000 ITERATIONS                                3 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:       735992 TO   759048
PROJECTED ANSWERS:            1607 TO     2877

L14           3 SEA SSS SAM L12 AND L10 NOT L11

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L15   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L16   SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505 (amended).str

L17     STRUCTURE UPLOADED
```

```
=> que L17 AND L15 NOT L16

L18  QUE L17 AND L15 NOT L16

=> d l18
L18 HAS NO ANSWERS
L15             SCR 1839
L16             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L17             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L18             QUE  L17 AND L15 NOT L16


=> s l18 sss sam
SAMPLE SEARCH INITIATED 10:29:02 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  37376 TO ITERATE

  2.7% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:       735992 TO   759048
PROJECTED ANSWERS:               0 TO        0

L19           0 SEA SSS SAM L17 AND L15 NOT L16

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L20   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L21   SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505 (examples).str

L22     STRUCTURE UPLOADED

=> que L22 AND L20 NOT L21

L23  QUE L22 AND L20 NOT L21

=> d l23
L23 HAS NO ANSWERS
L20             SCR 1839
L21             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L22             STR
```

```
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L23             QUE  L22 AND L20 NOT L21


=> s l23 sss sam
SAMPLE SEARCH INITIATED 10:33:37 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    8790 TO ITERATE

 11.4% PROCESSED    1000 ITERATIONS                                 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       170183 TO   181417
PROJECTED ANSWERS:               1 TO      352

L24           1 SEA SSS SAM L22 AND L20 NOT L21

=> s l23 sss ful
FULL SEARCH INITIATED 10:33:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 176029 TO ITERATE

100.0% PROCESSED  176029 ITERATIONS                             243 ANSWERS
SEARCH TIME: 00.00.03

L25         243 SEA SSS FUL L22 AND L20 NOT L21

=> s l25
L26           6 L25

=> d l26 1-6 bib,ab,hitstr
```

L26 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:412801 CAPLUS
DN 139:245782
TI Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease
IN Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy
PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SO PCT Int. Appl., 1243 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	WO 2003040096	A2	20030515	WO 2002-US36072	20021108
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2001-337122P	P	20011108		
	US 2001-344086P	P	20011228		
	US 2002-345635P	P	20020103		
	WO 2002-US36072	A	20021108		

OS MARPAT 139:245782
AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO2, (un)substituted NH; R4 = alkyl, haloalkyl, hydroxyalkyl, etc.; R5 = R6X (wherein X = CO, SO2, (un)substituted CH2; R6 = (un)substituted Ph, naphthyl, indanyl, etc.); R25 = H, alkyl, alkoxy, etc.] which have activity as inhibitors of .beta.-secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepd. E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC50 of < 20 .mu.M in cell free

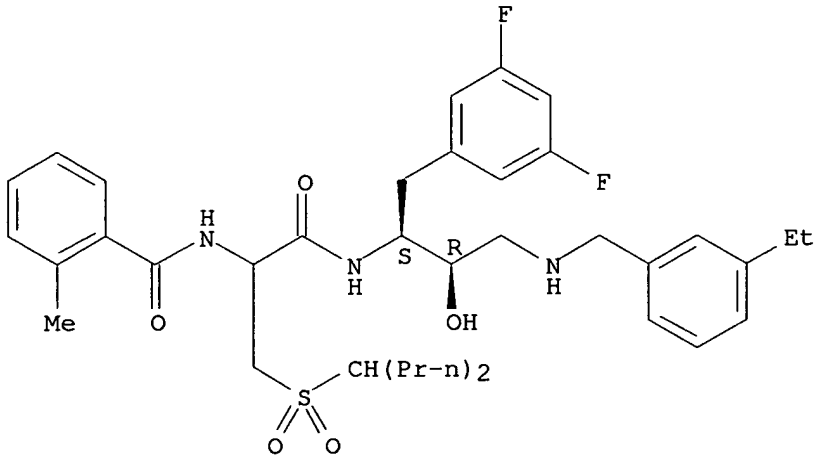
inhibition assay utilizing a synthetic APP substrate. This is a Part 2 of 1-2 series.

IT **477792-38-4P 477792-40-8P 477792-42-0P 477792-43-1P 477792-44-2P 477792-45-3P 477792-47-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

RN 477792-38-4 CAPLUS

CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

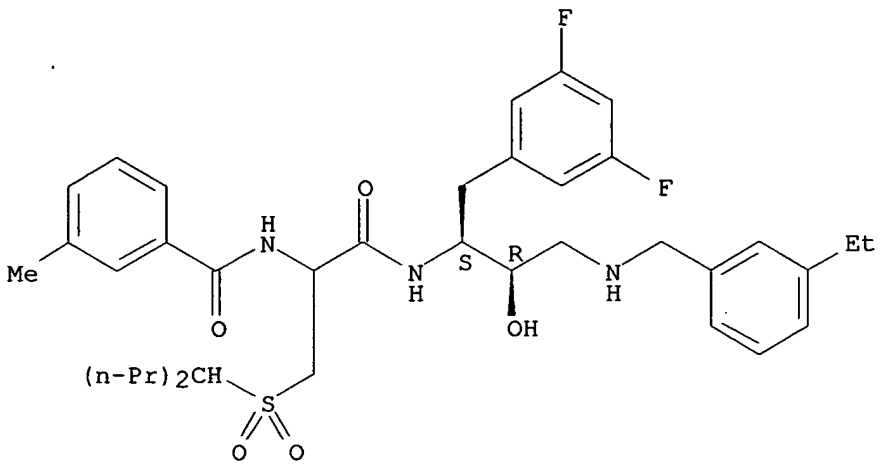


● HCl

RN 477792-40-8 CAPLUS

CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

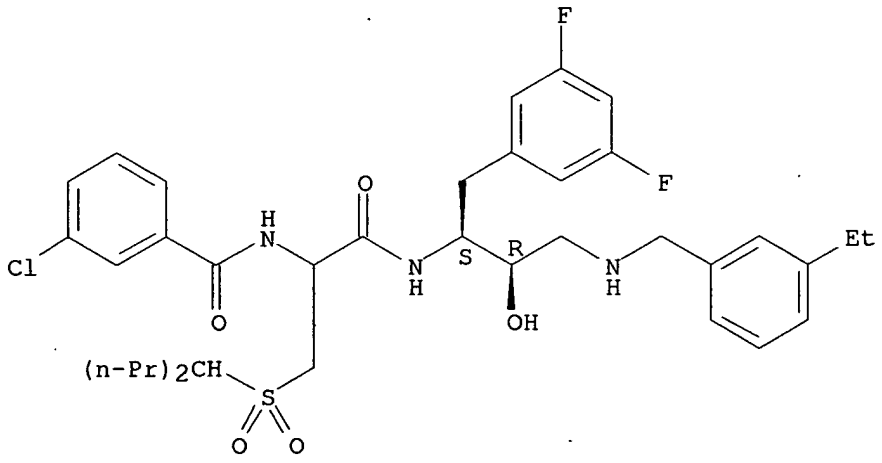
Absolute stereochemistry.



● HCl

RN 477792-42-0 CAPLUS
CN Benzamide, 3-chloro-N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

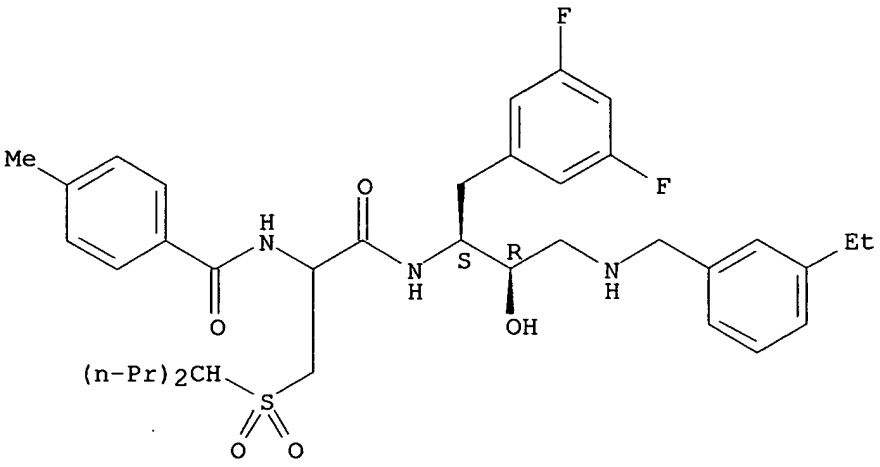
Absolute stereochemistry.



● HCl

RN 477792-43-1 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

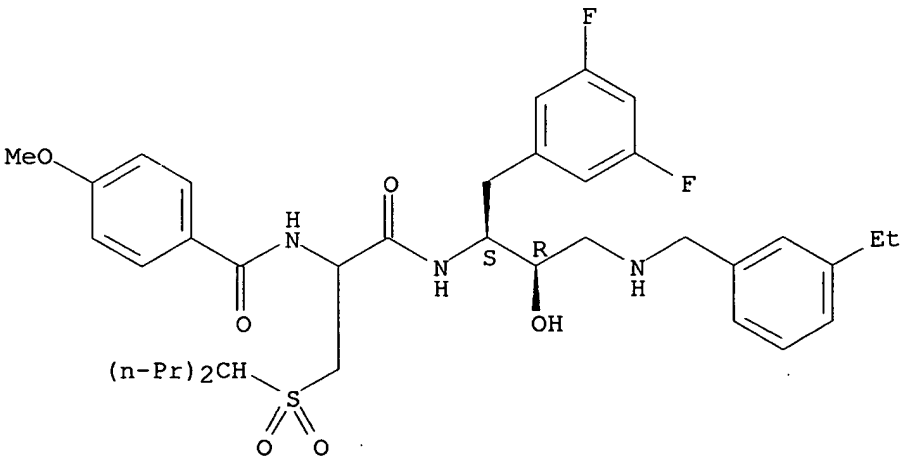
Absolute stereochemistry.



● HCl

RN 477792-44-2 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-methoxy-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

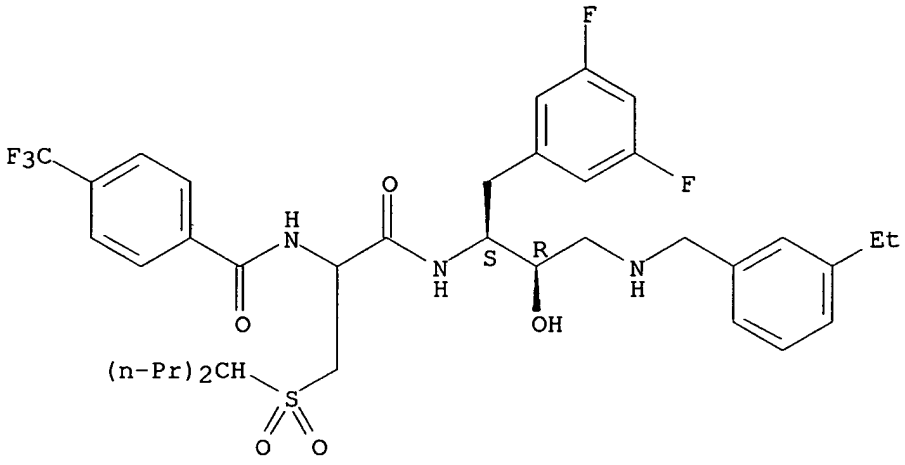


● HCl

RN 477792-45-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-

propylbutyl)sulfonyl]methyl]ethyl]-4-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

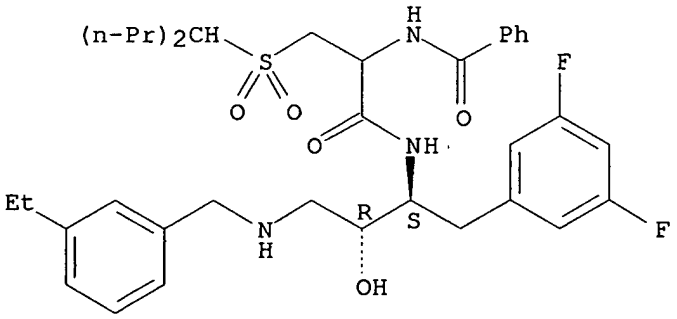
Absolute stereochemistry.



● HCl

RN 477792-47-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:376819 CAPLUS
DN 138:385173
TI Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease
IN Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy
PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SO PCT Int. Appl., 1243 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003040096	A2	20030515	WO 2002-US36072	20021108
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 2001-337122P	P	20011108		
	US 2001-344086P	P	20011228		
	US 2002-345635P	P	20020103		
	WO 2002-US36072	A	20021108		

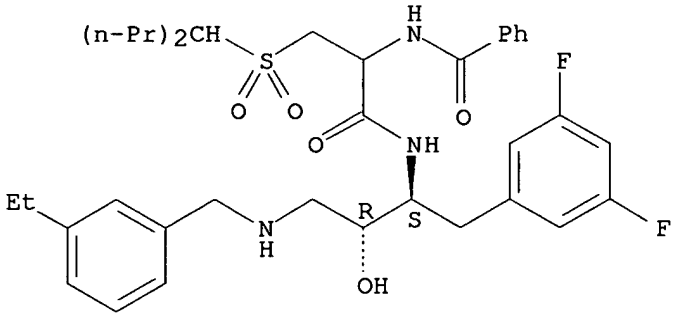
OS MARPAT 138:385173
AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO2, (un)substituted NH; R4 = alkyl, haloalkyl, hydroxyalkyl, etc.; R5 = R6X (wherein X = CO, SO2, (un)substituted CH2; R6 = (un)substituted Ph, naphthyl, indanyl, etc.); R25 = H, alkyl, alkoxy, etc.] which have activity as inhibitors of .beta.-secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepd. E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC50 of < 20 .mu.M in cell free

inhibition assay utilizing a synthetic APP substrate. This is a Part 1 of 1-2 series.

IT **477792-47-5P 477794-41-5P 477794-42-6P**
477794-43-7P 477794-44-8P 477794-45-9P
477794-46-0P 527712-74-9P 527712-76-1P
527712-78-3P 527712-81-8P 527712-83-0P
527712-87-4P 527715-44-2P 527715-46-4P
527717-43-7P 527733-82-0P 527735-34-8P
527735-54-2P 527735-55-3P 527735-58-6P
527735-59-7P 527735-62-2P 527735-63-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

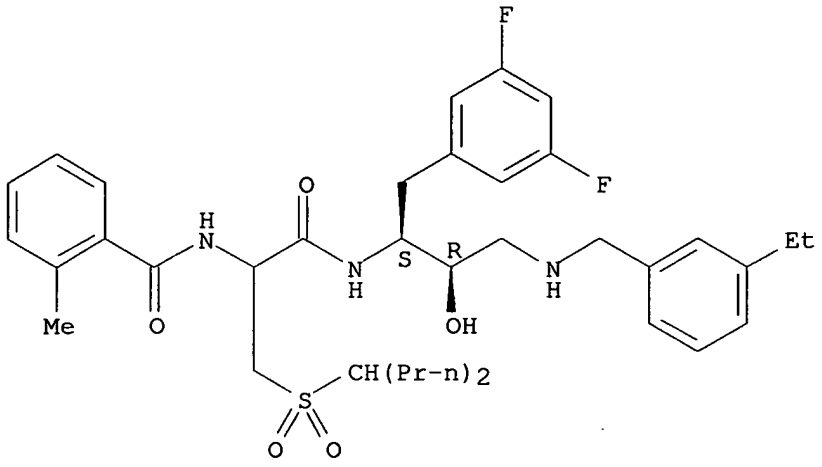
RN 477792-47-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



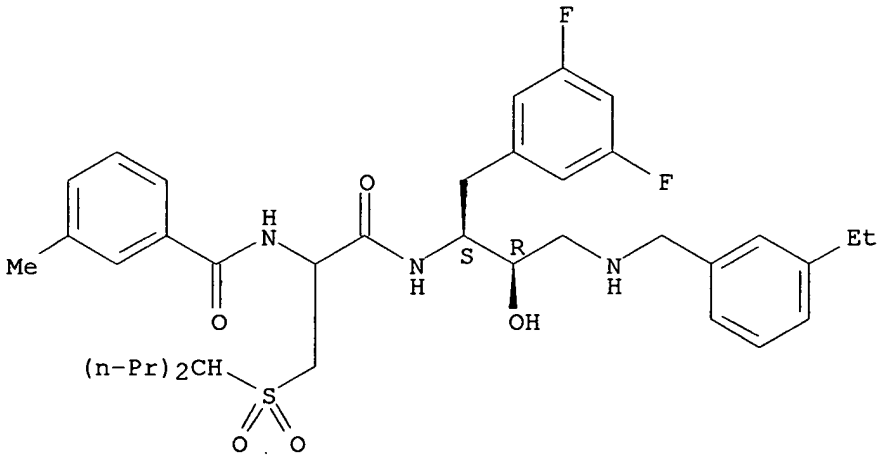
RN 477794-41-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



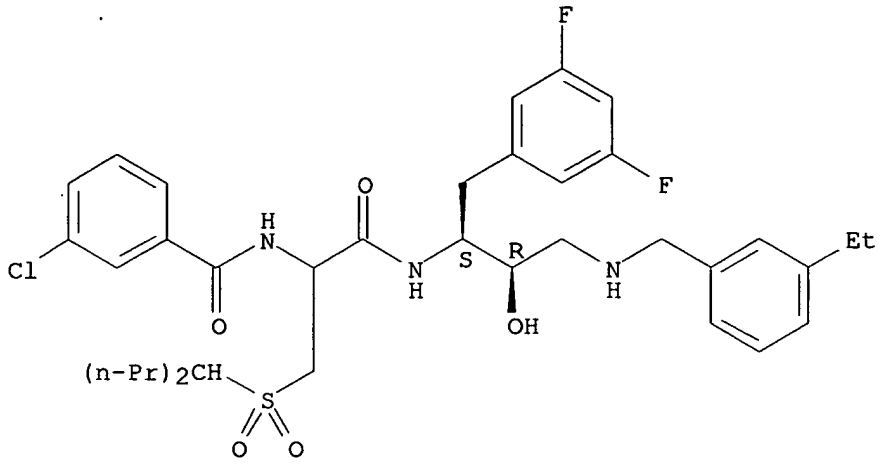
RN 477794-42-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



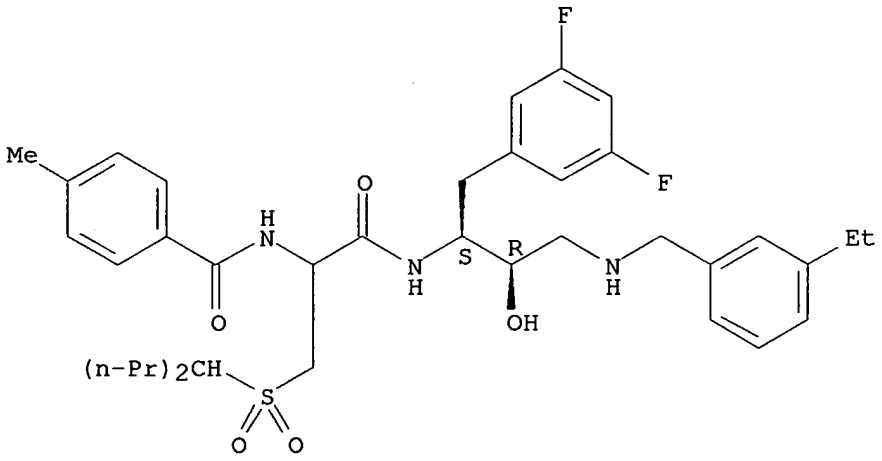
RN 477794-43-7 CAPLUS
CN Benzamide, 3-chloro-N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



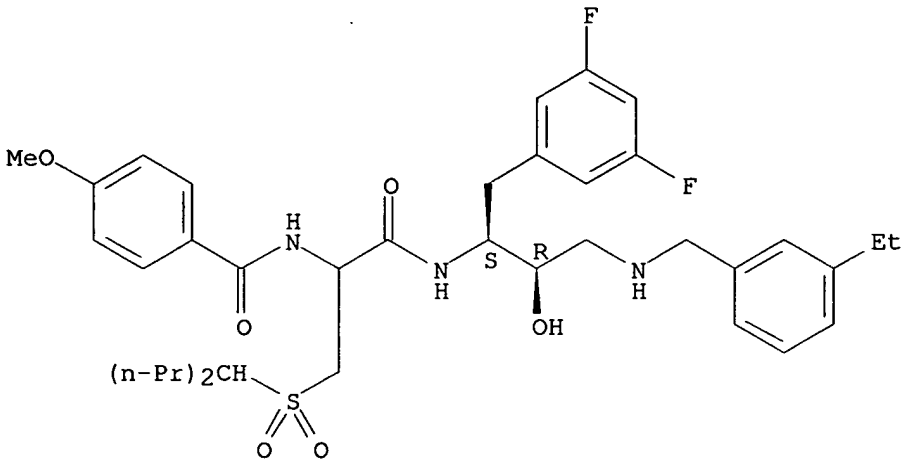
RN 477794-44-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



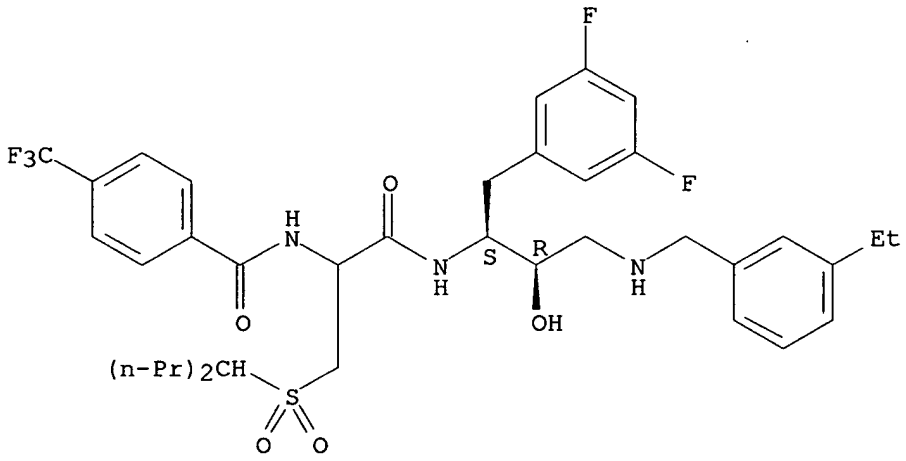
RN 477794-45-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl}ethyl]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

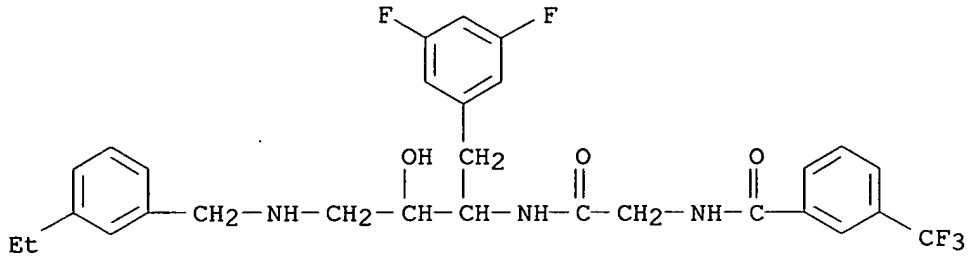


RN 477794-46-0 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

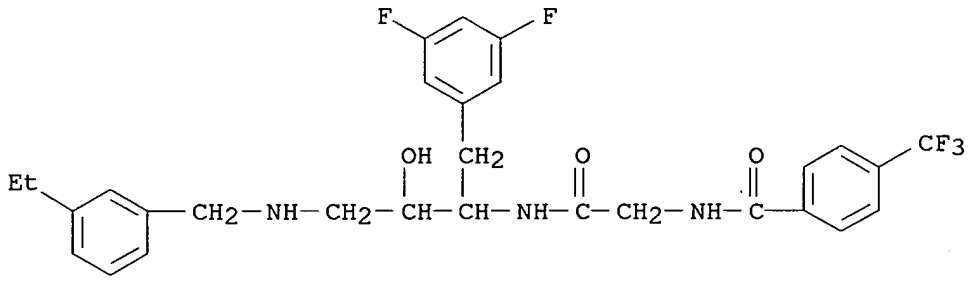
Absolute stereochemistry.



RN 527712-74-9 CAPLUS
CN Benzamide, N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 527712-76-1 CAPLUS
CN Benzamide, N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)



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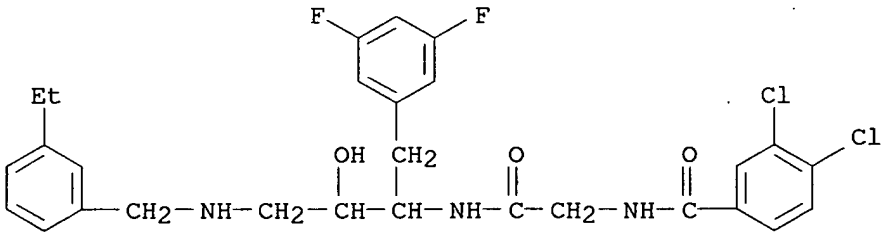
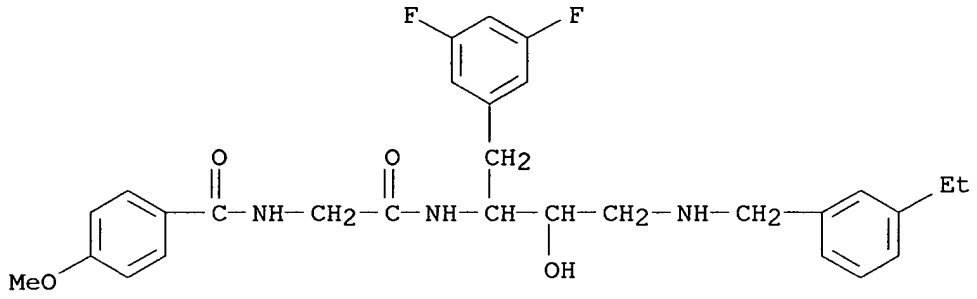
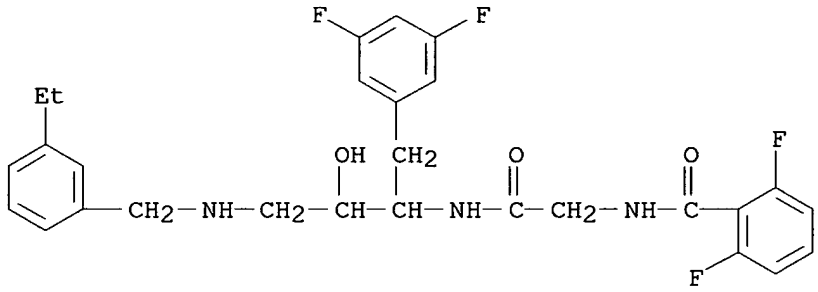
CN Benzamide, 3,4-dichloro-N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



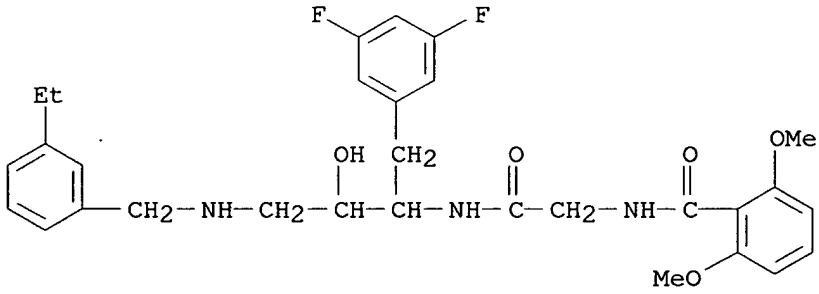
RN 527712-81-8 CAPLUS
CN Benzamide, N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-4-methoxy- (9CI) (CA INDEX NAME)



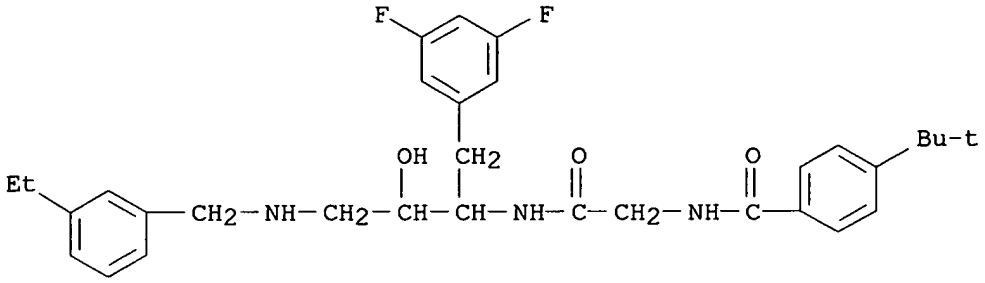
RN 527712-83-0 CAPLUS
CN Benzamide, N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-2,6-difluoro- (9CI) (CA INDEX NAME)



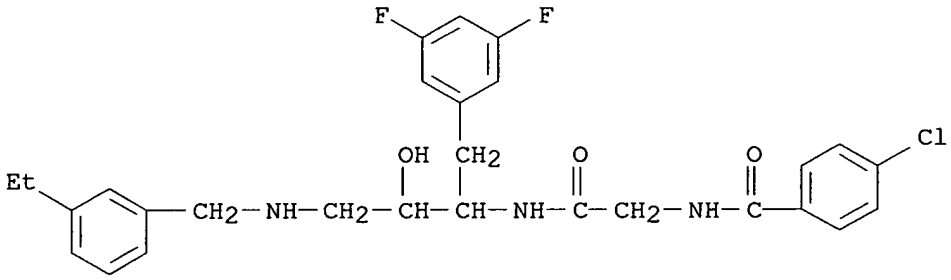
RN 527712-87-4 CAPLUS
CN Benzamide, N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-2,6-dimethoxy- (9CI) (CA INDEX NAME)



RN 527715-44-2 CAPLUS
CN Benzamide, N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-4-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

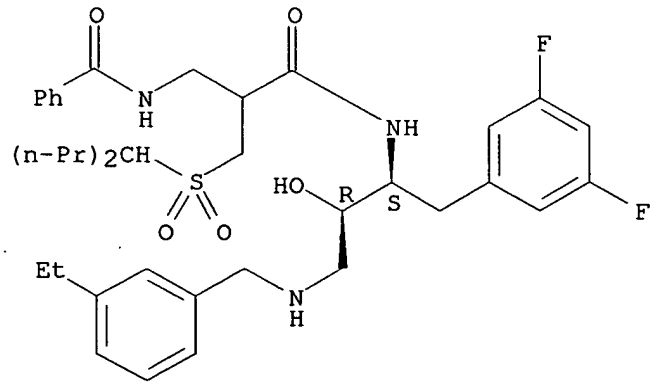


RN 527715-46-4 CAPLUS
CN Benzamide, 4-chloro-N-[2-[[1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



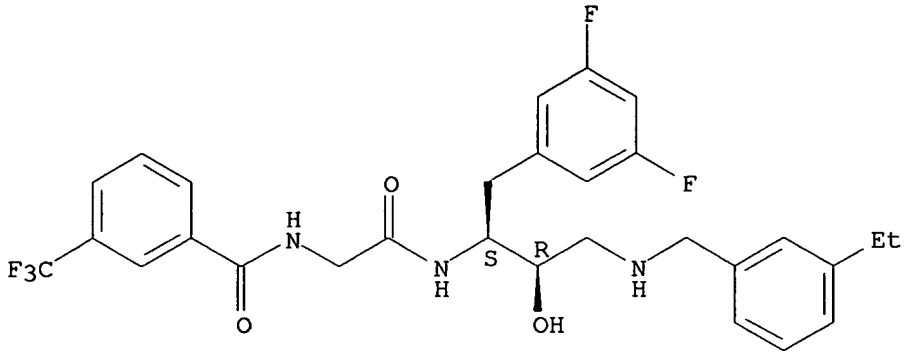
RN 527717-43-7 CAPLUS
CN Benzamide, N-[3-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-3-oxo-2-[[(1-propylbutyl)sulfonyl]methyl]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



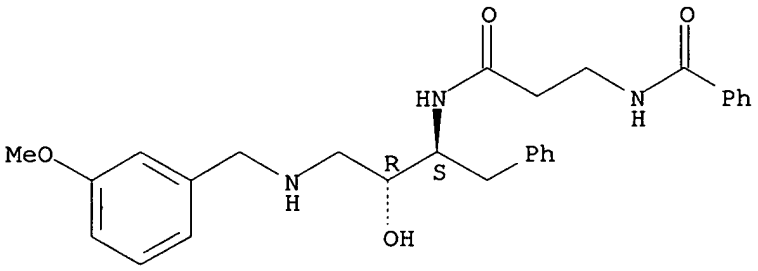
RN 527733-82-0 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



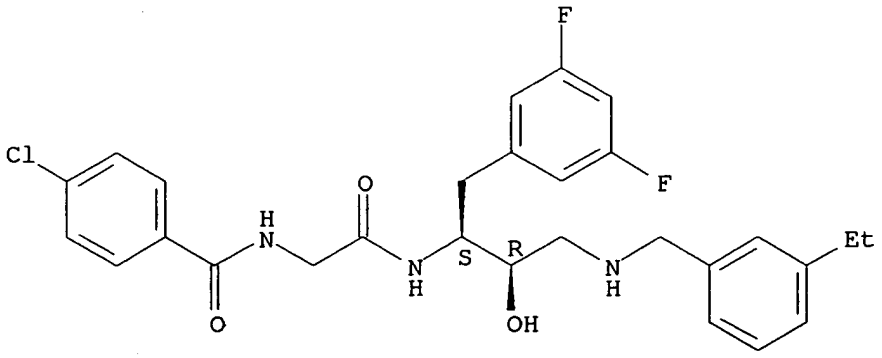
RN 527735-34-8 CAPLUS
CN Benzamide, N-[3-[[(1S,2R)-2-hydroxy-3-[[(3-methoxyphenyl)methyl]amino]-1-(phenylmethyl)propyl]amino]-3-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 527735-54-2 CAPLUS
CN Benzamide, 4-chloro-N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

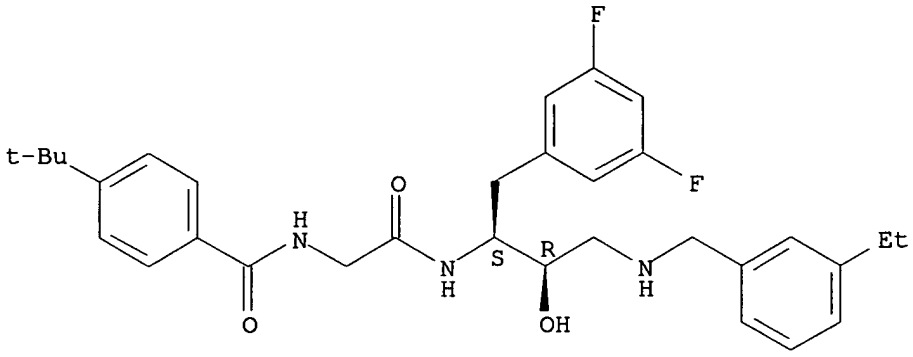
Absolute stereochemistry.



RN 527735-55-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-

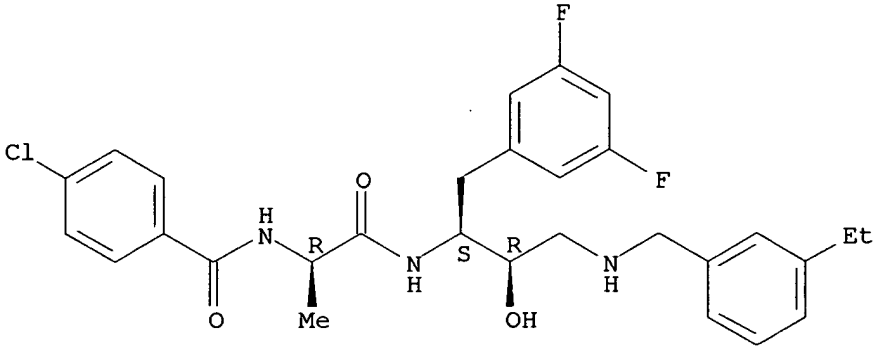
ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-4-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



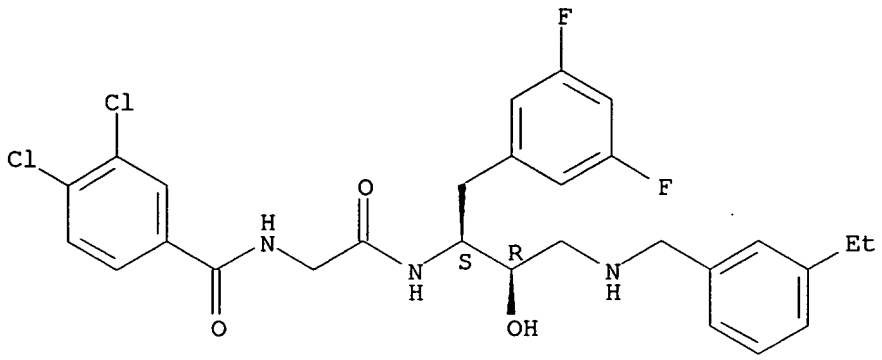
RN 527735-58-6 CAPLUS
CN Benzamide, 4-chloro-N-[(1R)-2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-1-methyl-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



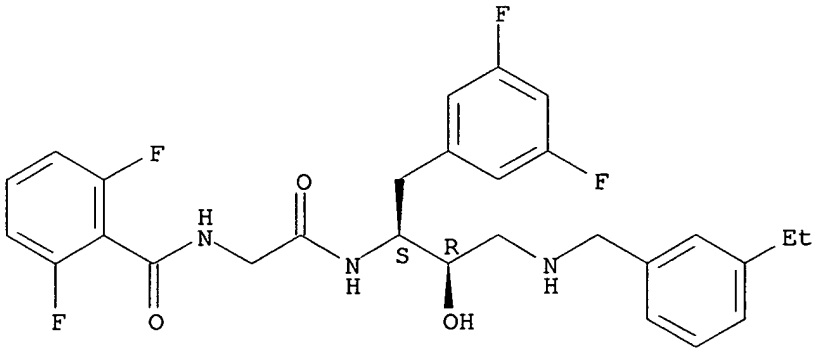
RN 527735-59-7 CAPLUS
CN Benzamide, 3,4-dichloro-N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



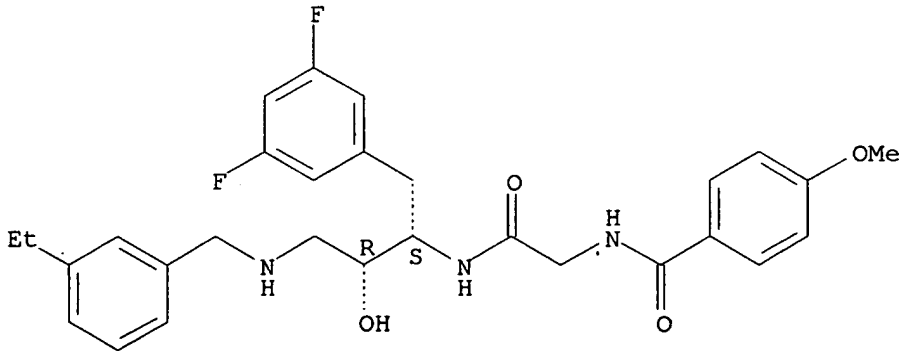
RN 527735-62-2 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-2,6-difluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 527735-63-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxoethyl]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:946261 CAPLUS
DN 138:14180
TI Preparation of peptide-related hydroxyalkylamines for pharmaceutical use in the treatment of Alzheimer's disease
IN Freskos, John; Aquino, Jose; Brown, David L.; Fang, Larry; Fobian, Yvette M.; Gailunas, Andrea; Guinn, Ashley; Varghese, John; Romero, Arthur Glenn; Tucker, John; Tung, Jay; Walker, Donald
PA Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company
SO PCT Int. Appl., 360 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002098849	A2	20021212	WO 2002-US17698	20020531
	WO 2002098849	A3	20031113		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003166717	A1	20030904	US 2002-160777	20020531
PRAI	US 2001-295332P	P	20010601		
	US 2001-332639P	P	20011119		
	US 2001-343772P	P	20011228		

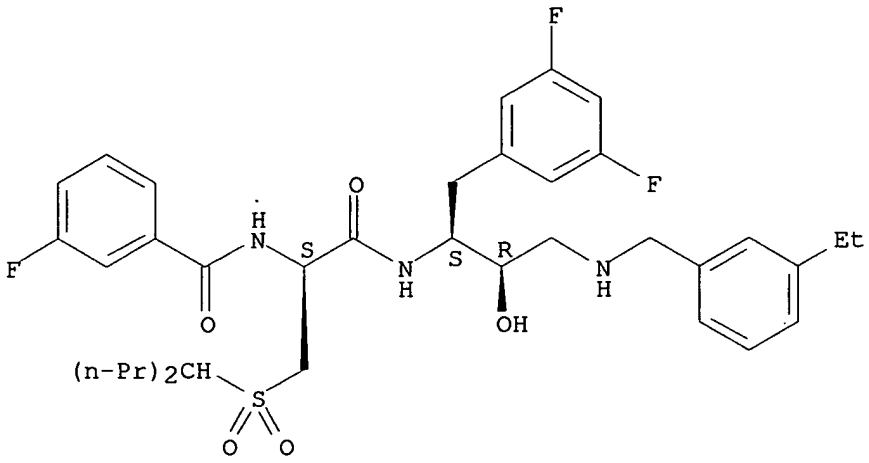
OS MARPAT 138:14180
AB Hydroxyalkylamines RNNR20CHR1CH(OH)CR2R3NR20Rc [RN is an acyl group of defined structure; R20 is H, (un)substituted alkyl, alkoxy, alkoxy-, hydroxy-, or haloalkyl, or -R26-R27, where R26 is CO, SO2, CO2, CONH, or alkylcarbamoyl and R27 is (un)substituted alkyl, alkoxy, arylalkyl, heterocycloalkyl, or heteroaryl; R1 is -(CH2)1-2-S(O)0-2-alkyl, (un)substituted alkyl, alkenyl, alkynyl, (hetero)aryl, heterocyclyl, etc.; R2, R3 are H or (un)substituted alkyl or CR2R3 is a 3-7 membered carbocycle in which one carbon atom is optionally replaced by O, S, SO2, or NRN-2; Rc is (un)substituted alkyl, (hetero)arylalkyl, heterocyclylalkyl, etc.] were prepd. for treating Alzheimer's disease and similar diseases. Synthetic procedures are given in examples and schemes. Several hundred products of the invention are listed in a table and in the claims, including S-butyl-N-1-[(1S,2R)-1-(3,5-difluorobenzyl)-3-[(3-ethylbenzyl)amino]-2-hydroxypropyl]-D-cysteinamide.
IT **477791-84-7P 477792-07-7P 477792-36-2P**
477792-37-3P 477792-38-4P 477792-39-5P
477792-40-8P 477792-41-9P 477792-42-0P
477792-43-1P 477792-44-2P 477792-45-3P
477792-47-5P 477792-52-2P 477794-10-8P
477794-39-1P 477794-40-4P 477794-41-5P
477794-42-6P 477794-43-7P 477794-44-8P
477794-45-9P 477794-46-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide-related hydroxyalkylamines for treatment of Alzheimer's disease)

RN 477791-84-7 CAPLUS

CN Benzamide, N-[(1S)-2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-fluoro-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

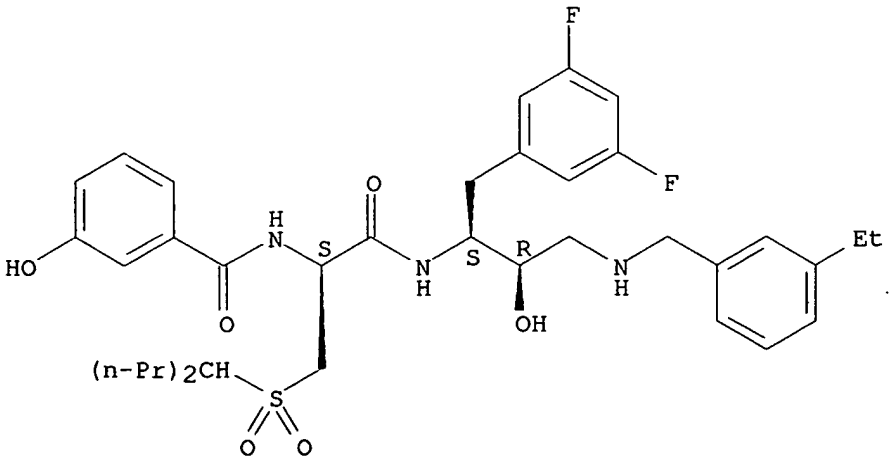


● HCl

RN 477792-07-7 CAPLUS

CN Benzamide, N-[(1S)-2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-hydroxy- (9CI) (CA INDEX NAME)

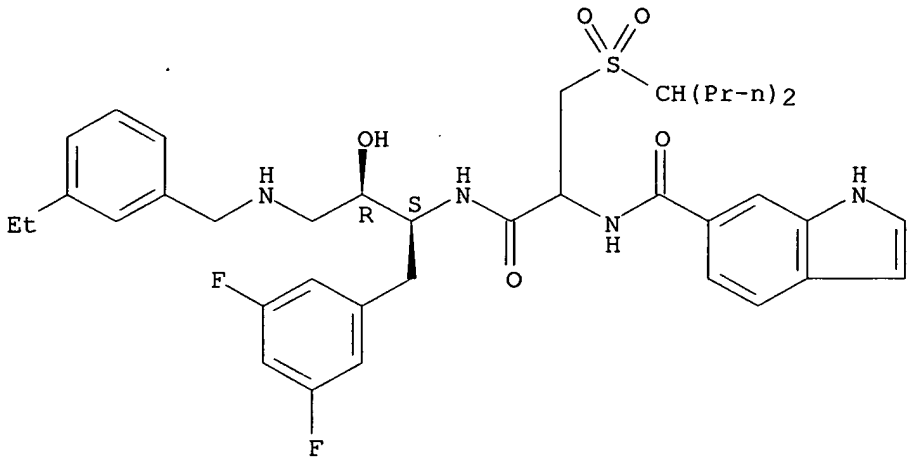
Absolute stereochemistry.



RN 477792-36-2 CAPLUS

CN 1H-Indole-6-carboxamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

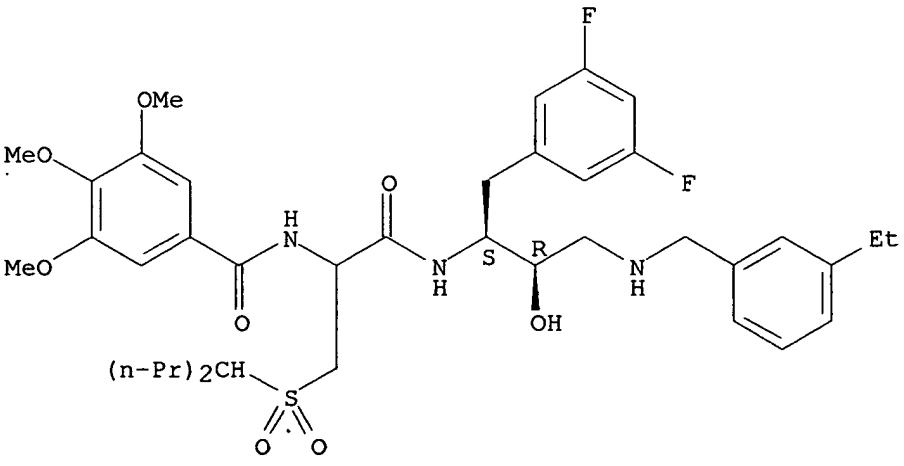


● HCl

RN 477792-37-3 CAPLUS

CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3,4,5-trimethoxy-, monohydrochloride (9CI) (CA INDEX NAME)

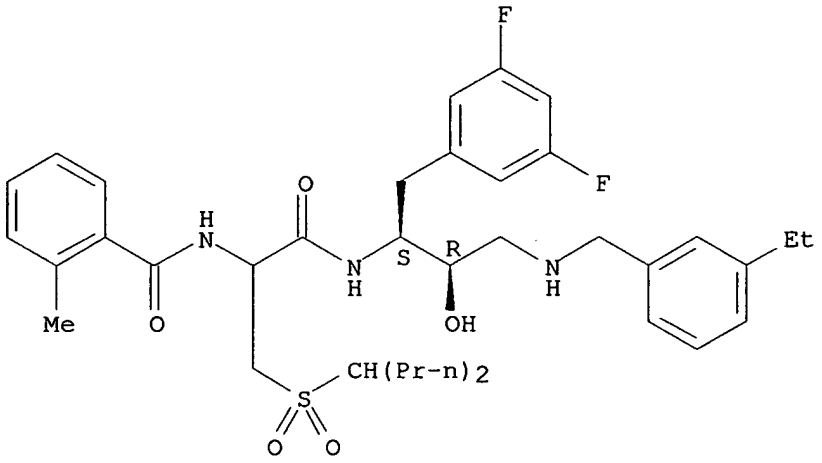
Absolute stereochemistry.



● HCl

RN 477792-38-4 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-2-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

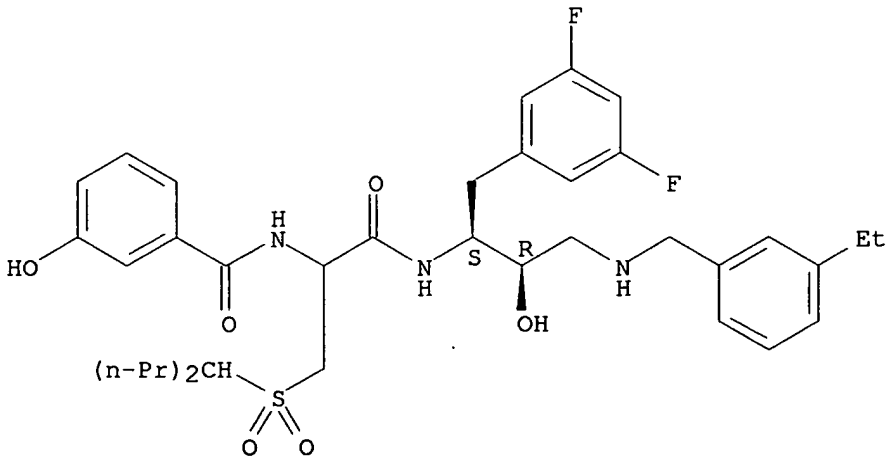
Absolute stereochemistry.



● HCl

RN 477792-39-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-hydroxy- (9CI) (CA INDEX NAME)

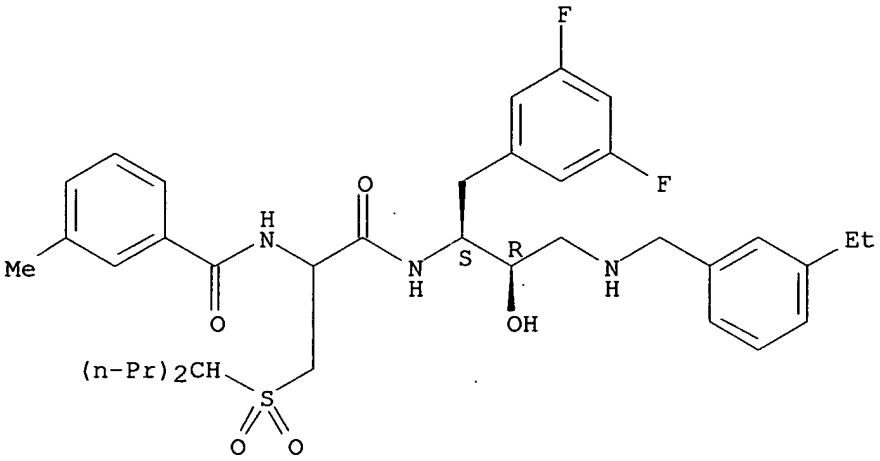
Absolute stereochemistry.



RN 477792-40-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-

ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

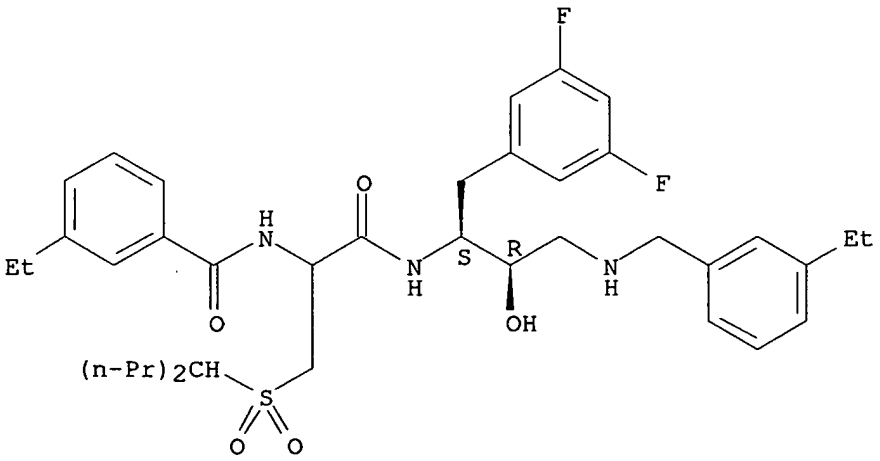
Absolute stereochemistry.



● HCl

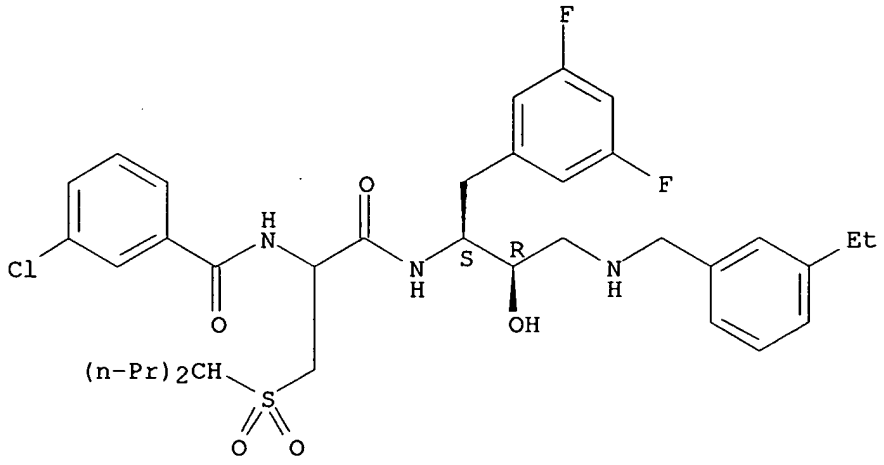
RN 477792-41-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-ethyl-, (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 477792-42-0 CAPLUS
CN Benzamide, 3-chloro-N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

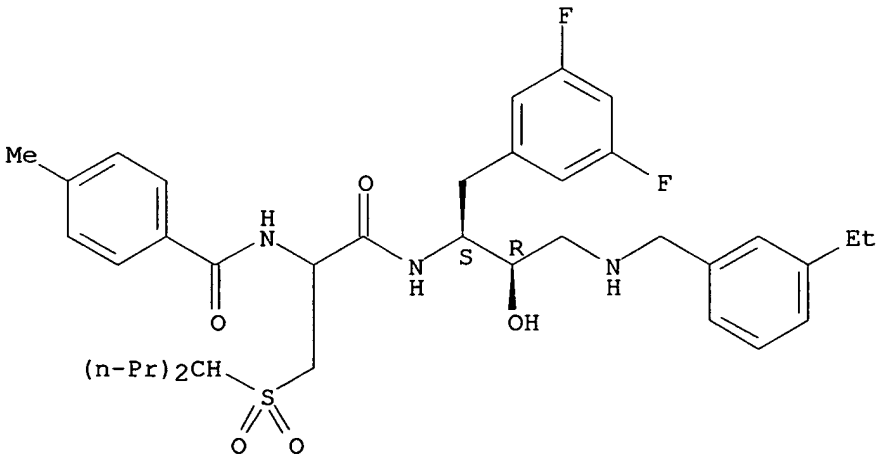
Absolute stereochemistry.



● HCl

RN 477792-43-1 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

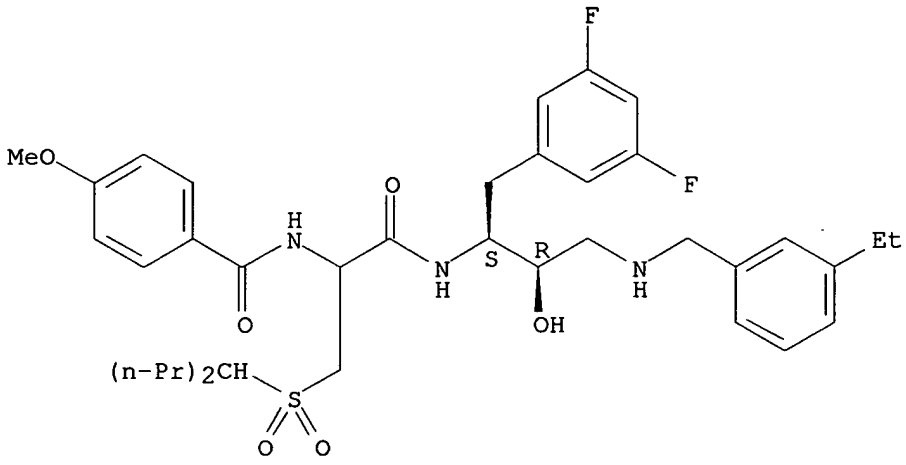


● HCl

RN 477792-44-2 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-

propylbutyl)sulfonyl]methyl]ethyl]-4-methoxy-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

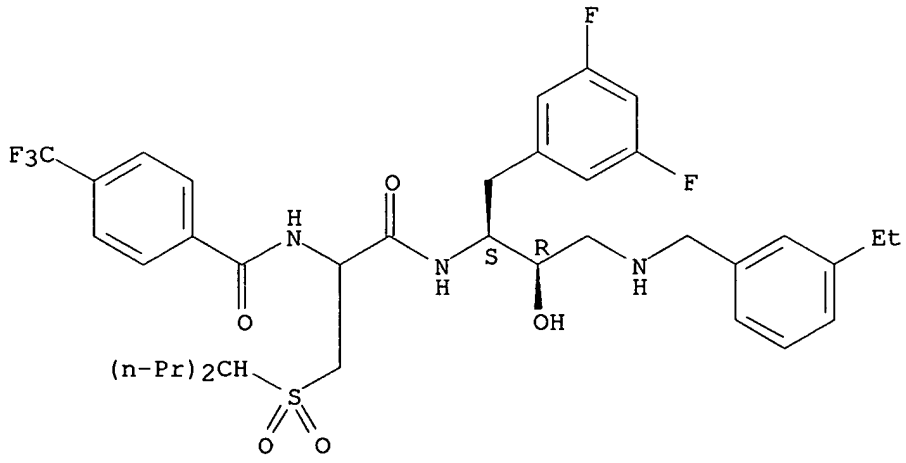


● HCl

RN 477792-45-3 CAPLUS

CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

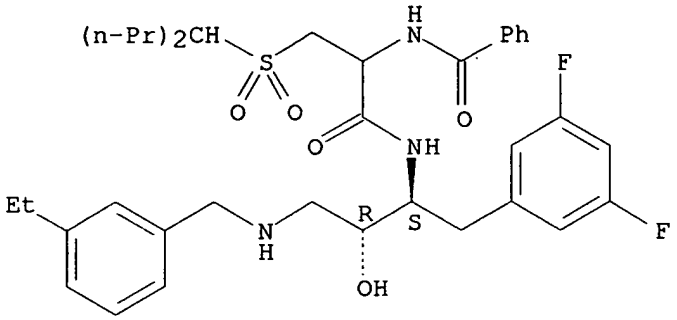


● HCl

RN 477792-47-5 CAPLUS

CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

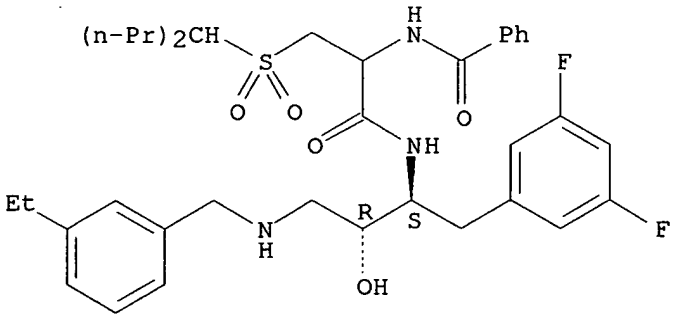


RN 477792-52-2 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

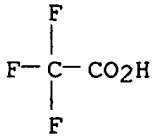
CRN 477792-47-5
CMF C36 H47 F2 N3 O5 S

Absolute stereochemistry.



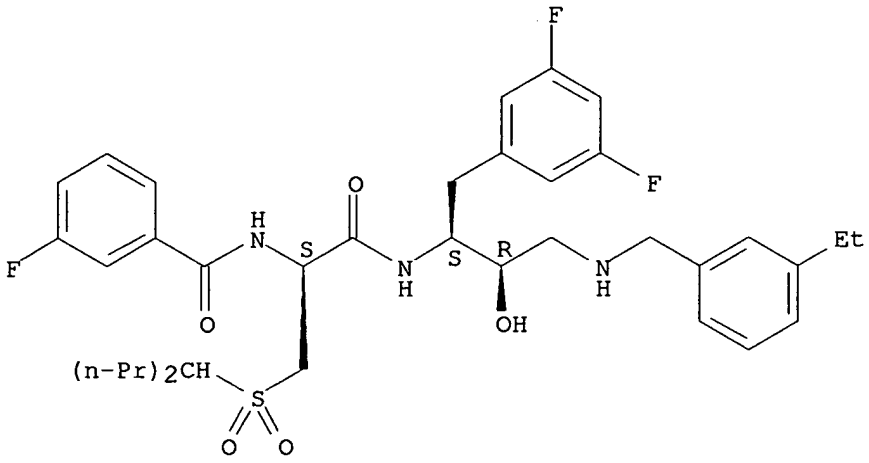
CM 2

CRN 76-05-1
CMF C2 H F3 O2



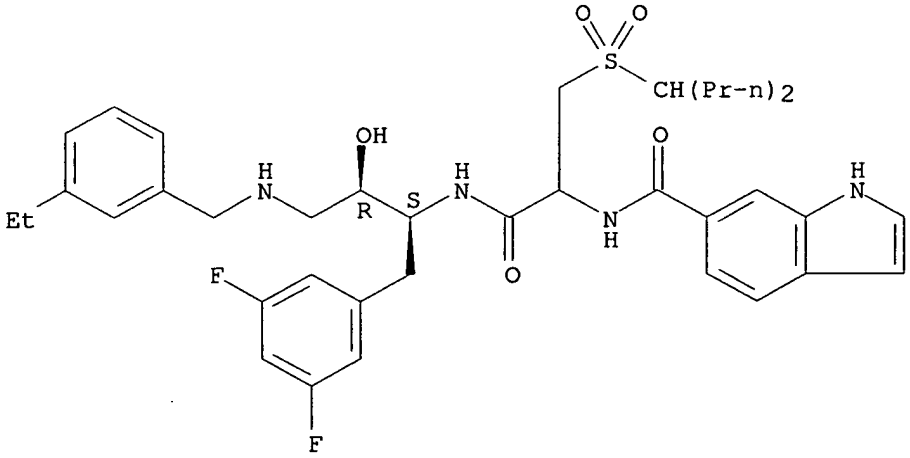
RN 477794-10-8 CAPLUS
CN Benzamide, N-[(1S)-2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-fluoro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



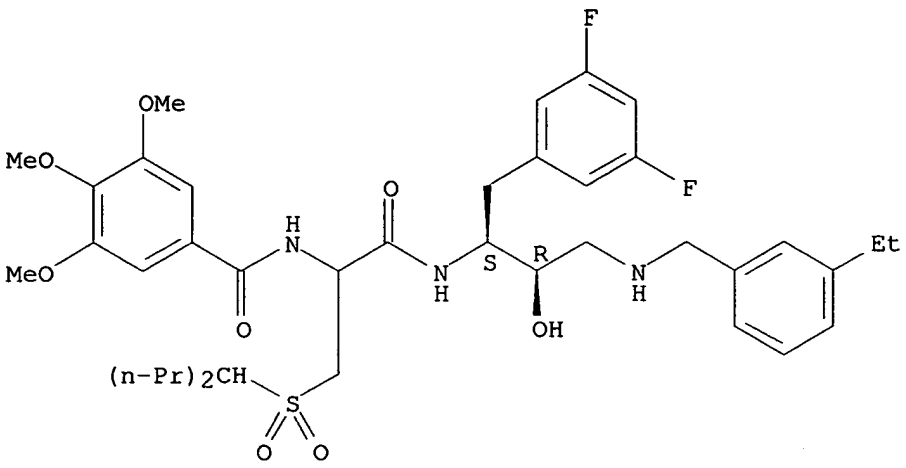
RN 477794-39-1 CAPLUS
CN 1H-Indole-6-carboxamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



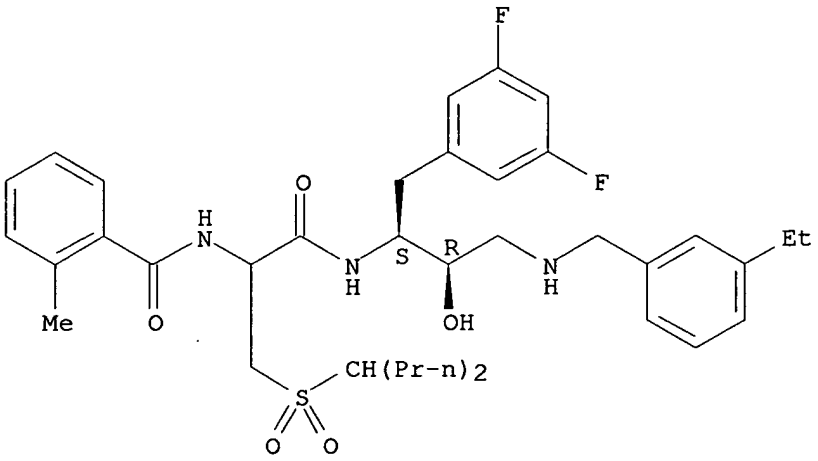
RN 477794-40-4 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3,4,5-trimethoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



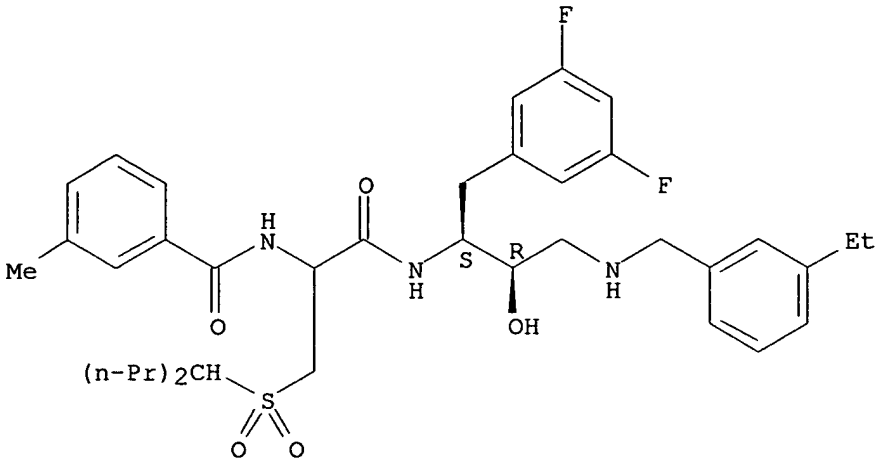
RN 477794-41-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-2-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



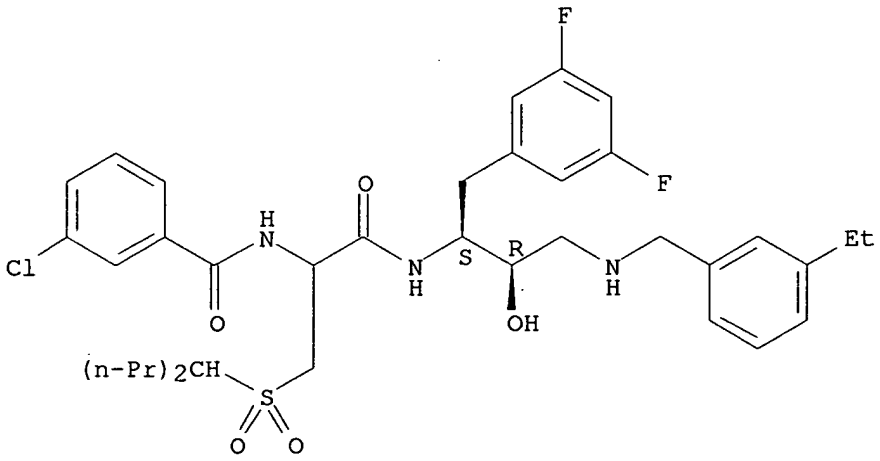
RN 477794-42-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-3-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



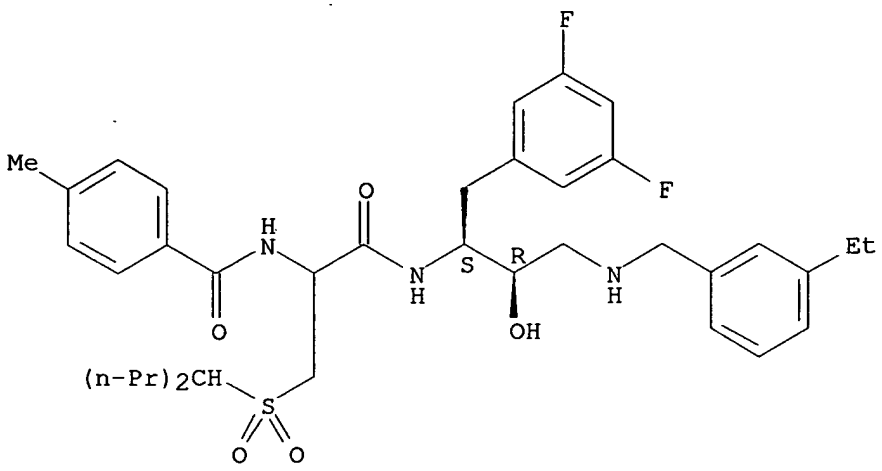
RN 477794-43-7 CAPLUS
CN Benzamide, 3-chloro-N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



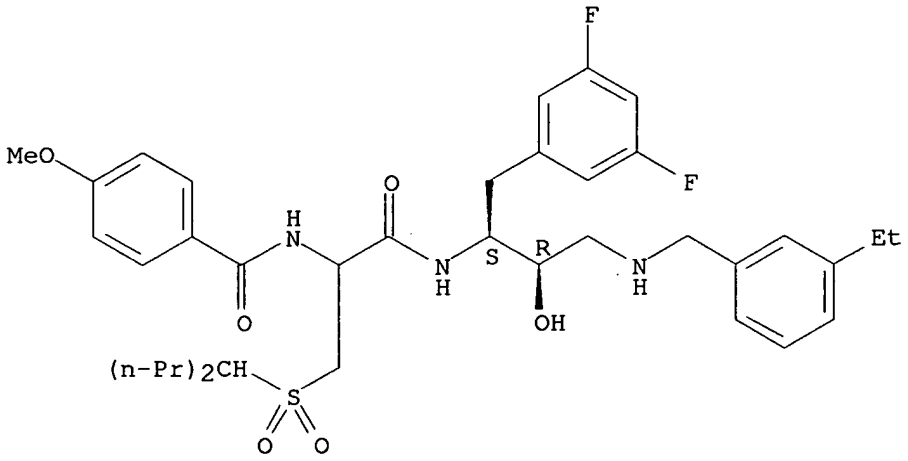
RN 477794-44-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



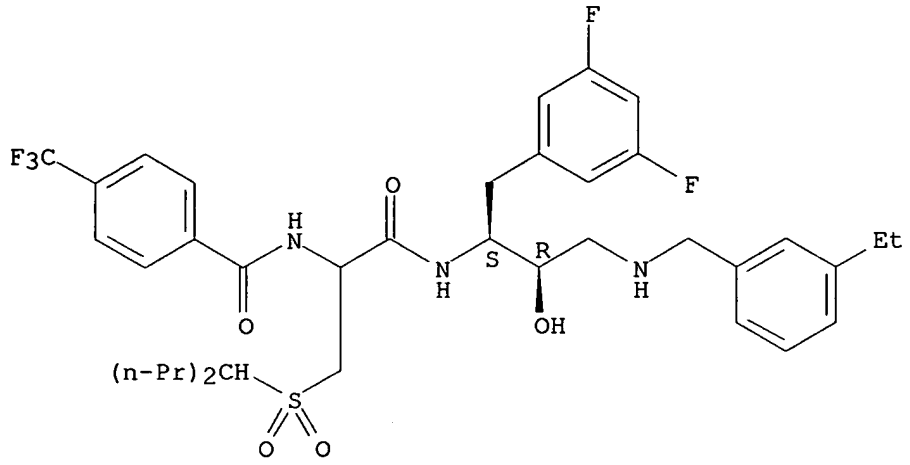
RN 477794-45-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 477794-46-0 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[(3-ethylphenyl)methyl]amino]-2-hydroxypropyl]amino]-2-oxo-1-[[(1-propylbutyl)sulfonyl]methyl]ethyl]-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

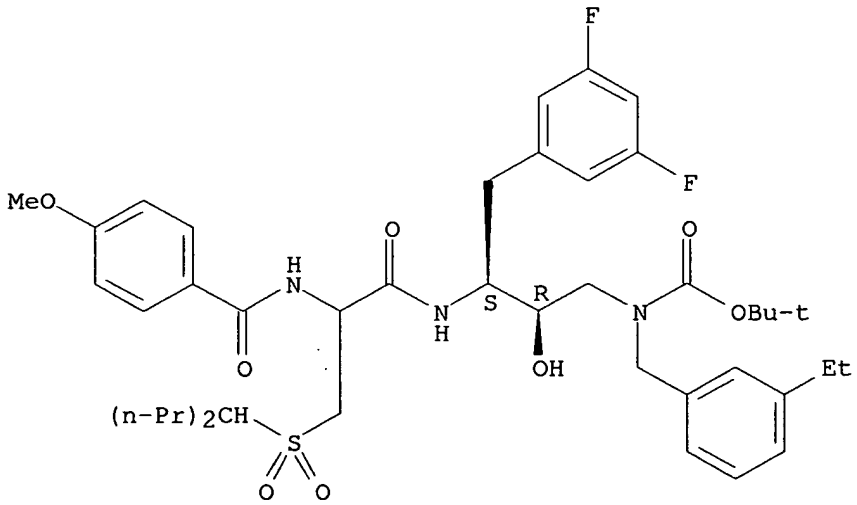


IT **477790-58-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of peptide-related hydroxyalkylamines for treatment of Alzheimer's disease)

RN 477790-58-2 CAPLUS

CN Carbamic acid, [(2R,3S)-4-(3,5-difluorophenyl)-2-hydroxy-3-[[2-[(4-methoxybenzoyl)amino]-1-oxo-3-[(1-propylbutyl)sulfonyl]propyl]amino]butyl][(3-ethylphenyl)methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L26 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:487516 CAPLUS
DN 137:63474
TI Preparation of amino acid-related diamines as modulators of chemokine receptor activity
IN Carter, Percy; Cherney, Robert
PA Bristol-Myers Squibb Pharma Company, USA
SO PCT Int. Appl., 375 pp.
CODEN: PIXXD2
DT Patent
LA English

Appl. PCT

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002050019	A2	20020627	WO 2001-US50619	20011220
	WO 2002050019	A3	20030313		
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	AU 2002041724	A5	20020701	AU 2002-41724	20011220
	US 2003060459	A1	20030327	US 2001-27505	20011220 ←
	EP 1351924	A2	20031015	EP 2001-988415	20011220
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PRAI	US 2000-256855P	P	20001220		
	WO 2001-US50619	W	20011220		

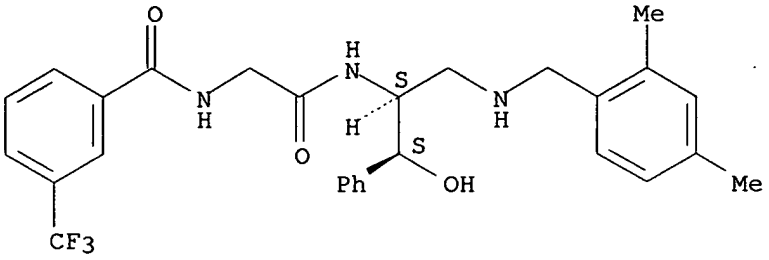
OS MARPAT 137:63474

AB Diamine compds. R1-X-CR6R7(CR8R9)m(CR10R11)lCR12R3NHCO(CR14R14a)nNR15-Z-R2 [Z = a bond, CONH, C(S)NH, SO2, SO2NH; X = NH, (cyclo)alkylimino, O, S, methyleneimino optionally substituted by (cyclo)alkyl; R1, R2 = (hetero)aryl; R3 = H, functionalized alkyl, (hetero)cyclyl; R6-R12 = alkyl, alkenyl, alkynyl, any group given for R3; R14, R14a = (un)substituted alkyl; n = 1 or 2; l, m = 0 or 1] or their pharmaceutically acceptable salt were prepd. as modulators of chemokine receptor activity for use in the treatment and prevention of asthma, multiple sclerosis, atherosclerosis, and rheumatoid arthritis. One hundred ninety-four diamines, e.g., Me (2S)-3-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]propanoate, were synthesized and claimed. All examples of the present invention have activity (IC50 = 50% at .ltorsim. 20 .mu.M) in the antagonism of MCP-1 binding to human PBMC (human peripheral blood mononuclear cells).

IT **439149-10-7P 439149-11-8P**
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)

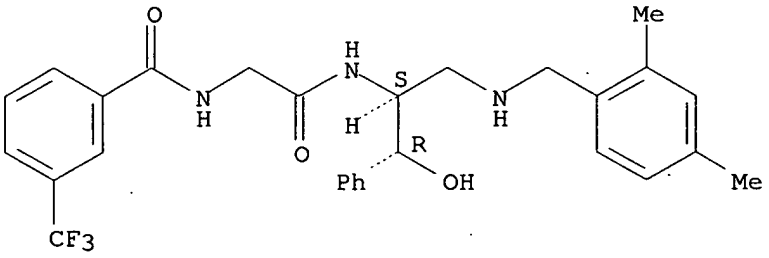
RN 439149-10-7 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



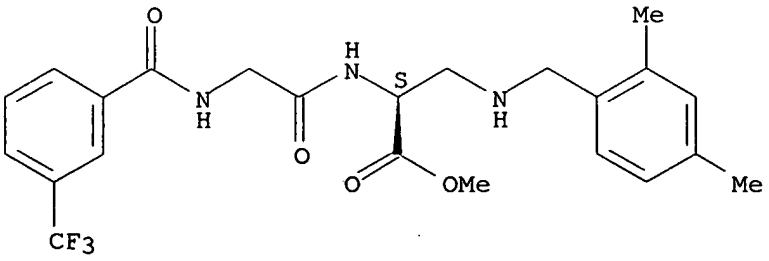
RN 439149-11-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



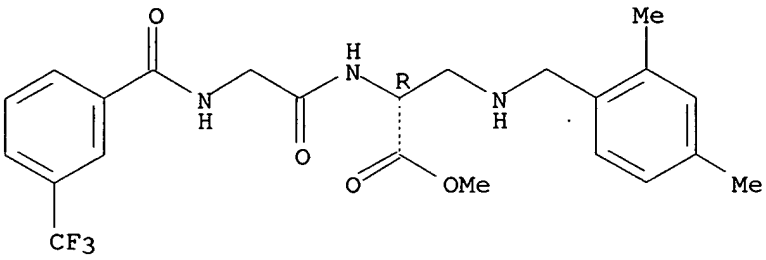
IT **439148-61-5P 439148-62-6P 439148-63-7P**
439148-76-2P 439148-85-3P 439148-98-8P
439149-02-7P 439149-18-5P 439149-47-0P
439150-06-8P 439150-30-8P 439150-38-6P
439150-42-2P 439150-44-4P 439150-52-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)
RN 439148-61-5 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



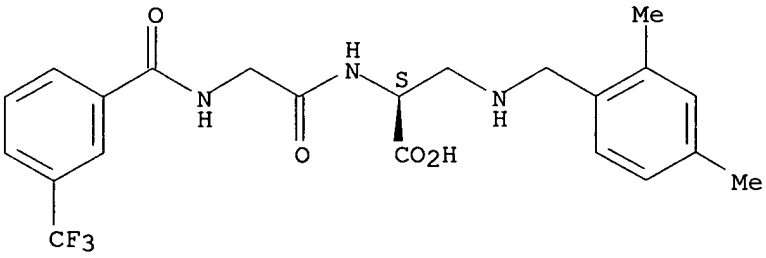
RN 439148-62-6 CAPLUS
CN D-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



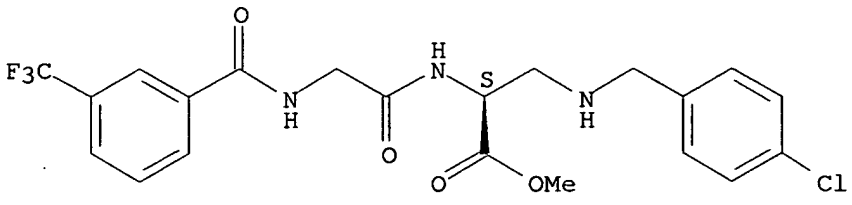
RN 439148-63-7 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



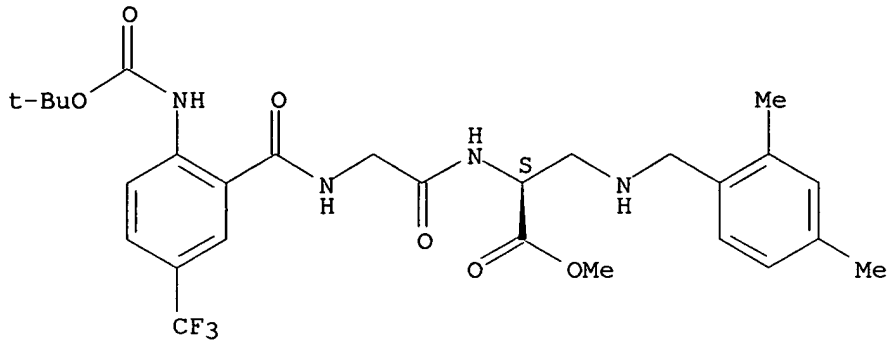
RN 439148-76-2 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-chlorophenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



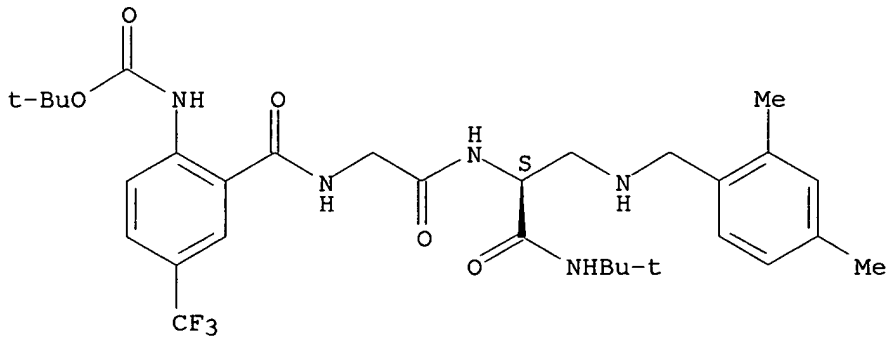
RN 439148-85-3 CAPLUS
CN L-Alanine, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



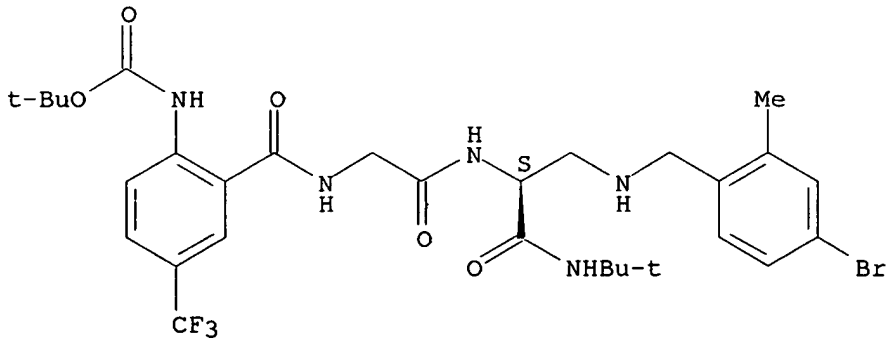
RN 439148-98-8 CAPLUS
CN L-Alaninamide, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439149-02-7 CAPLUS
CN L-Alaninamide, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

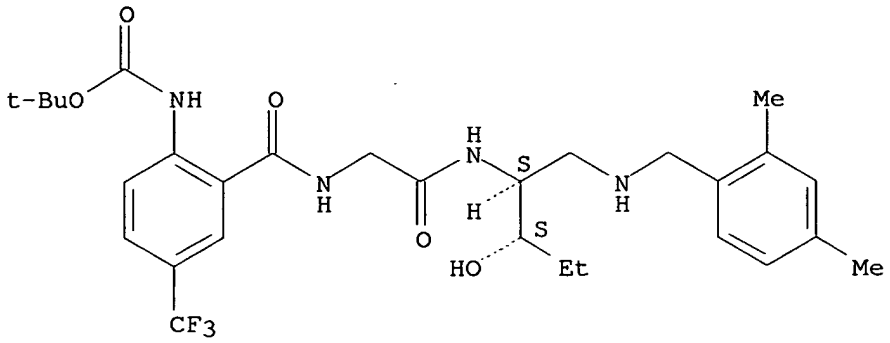
Absolute stereochemistry.



RN 439149-18-5 CAPLUS

CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-1-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

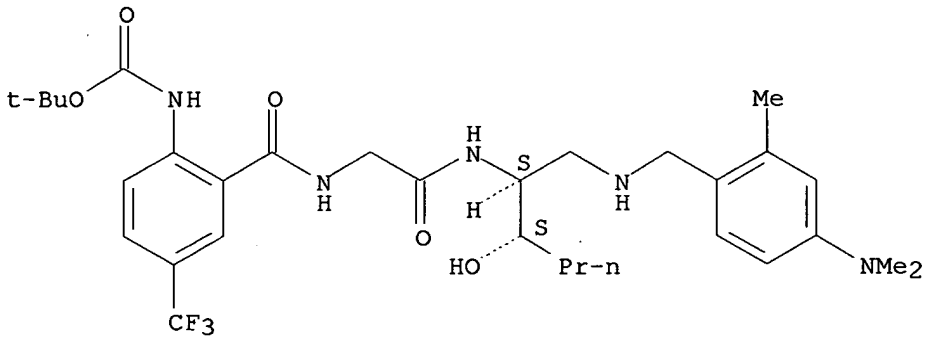
Absolute stereochemistry.



RN 439149-47-0 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[[4-(dimethylamino)-2-methylphenyl]methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

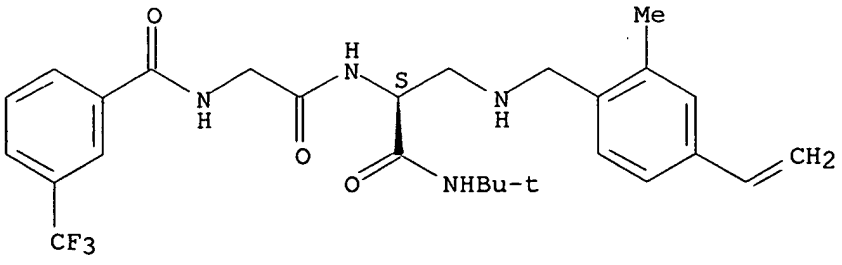
Absolute stereochemistry.



RN 439150-06-8 CAPLUS

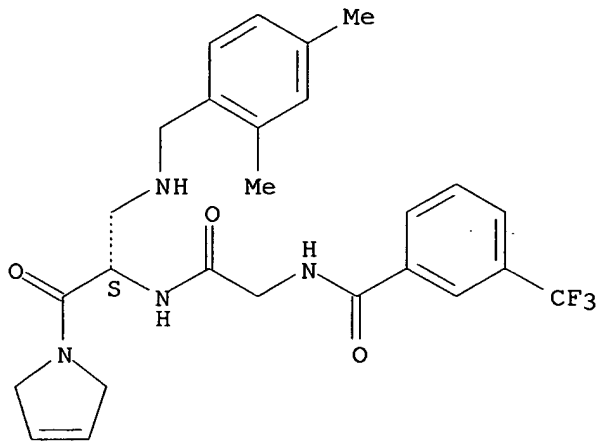
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-ethenyl-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



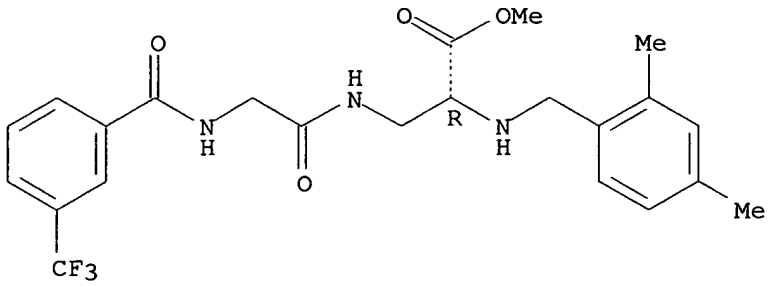
RN 439150-30-8 CAPLUS
CN Benzamide, N-[2-[[(1S)-2-(2,5-dihydro-1H-pyrrol-1-yl)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-oxoethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



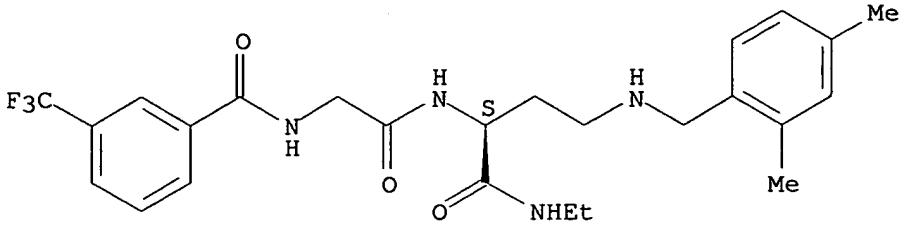
RN 439150-38-6 CAPLUS
CN .beta.-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-2-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



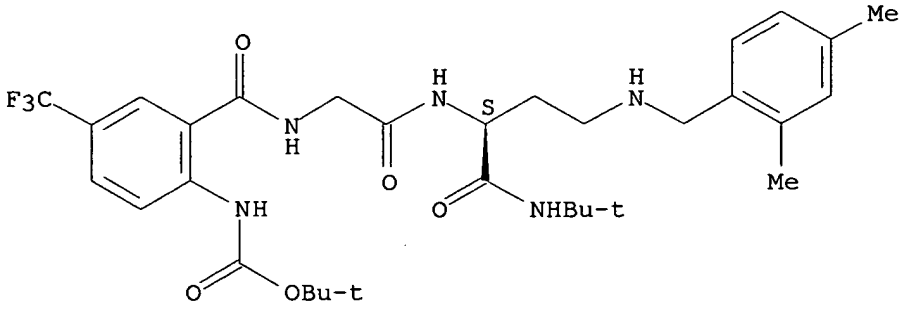
RN 439150-42-2 CAPLUS
CN Benzamide, N-[2-[[(1S)-3-[[(2,4-dimethylphenyl)methyl]amino]-1-[(ethylamino)carbonyl]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



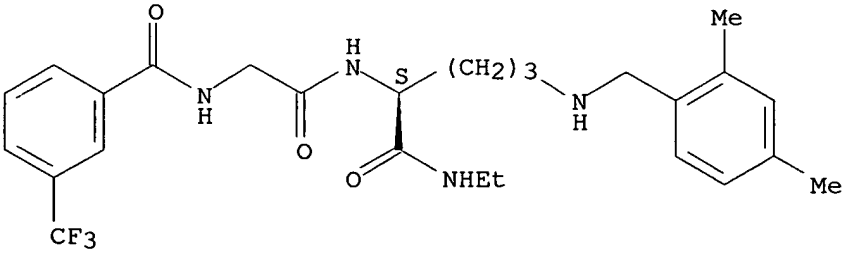
RN 439150-44-4 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(2,4-dimethylphenyl)methyl]amino]propyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439150-52-4 CAPLUS
CN L-Ornithinamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N5-[(2,4-dimethylphenyl)methyl]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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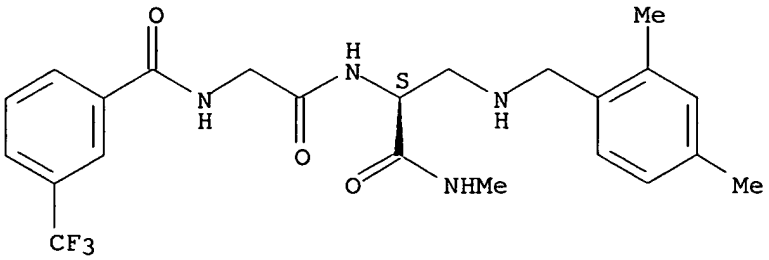
439150-17-1P 439150-18-2P 439150-19-3P
439150-20-6P 439150-21-7P 439150-22-8P
439150-23-9P 439150-24-0P 439150-25-1P
439150-26-2P 439150-27-3P 439150-28-4P
439150-29-5P 439150-31-9P 439150-32-0P
439150-33-1P 439150-34-2P 439150-35-3P
439150-36-4P 439150-37-5P 439150-39-7P
439150-40-0P 439150-41-1P 439150-43-3P
439150-45-5P 439150-46-6P 439150-47-7P
439150-48-8P 439150-49-9P 439150-50-2P
439150-51-3P 439150-53-5P 439150-54-6P
439150-55-7P 439150-56-8P 439150-57-9P
439150-58-0P 439150-65-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)

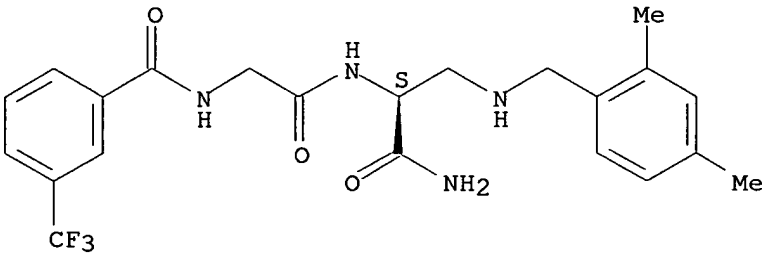
RN 439148-64-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



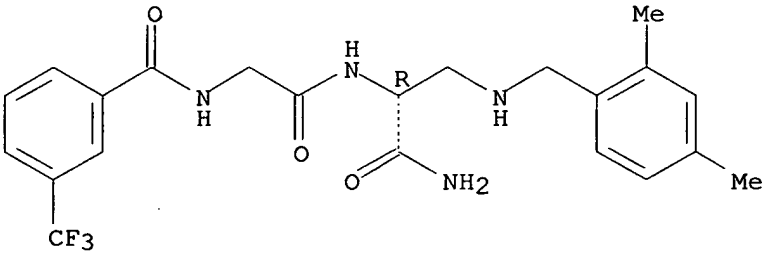
RN 439148-65-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



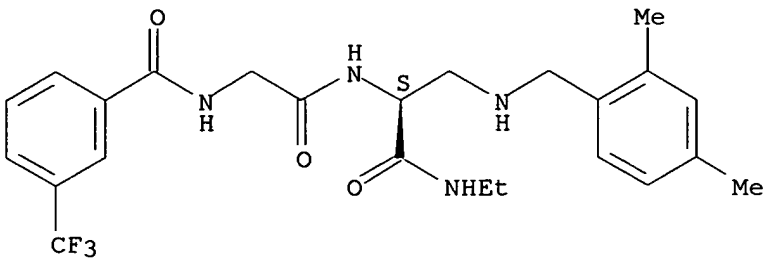
RN 439148-66-0 CAPLUS
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



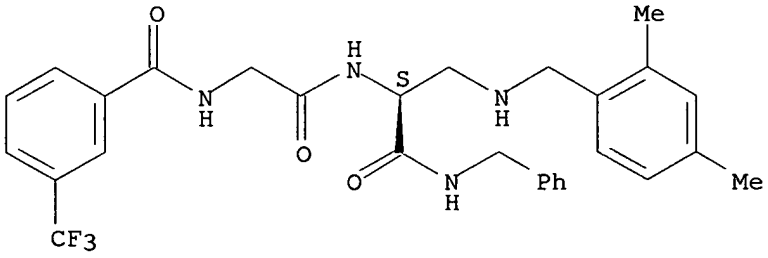
RN 439148-67-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



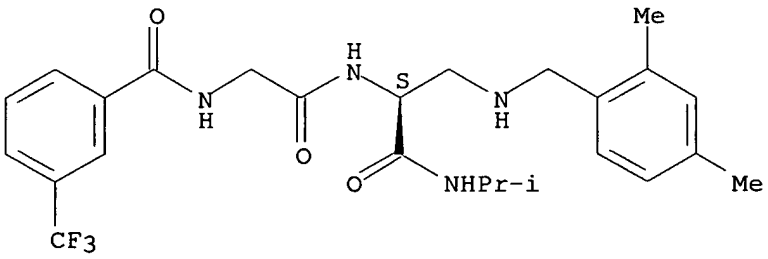
RN 439148-68-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



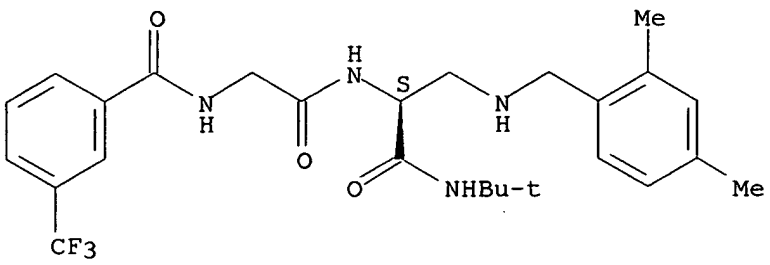
RN 439148-69-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



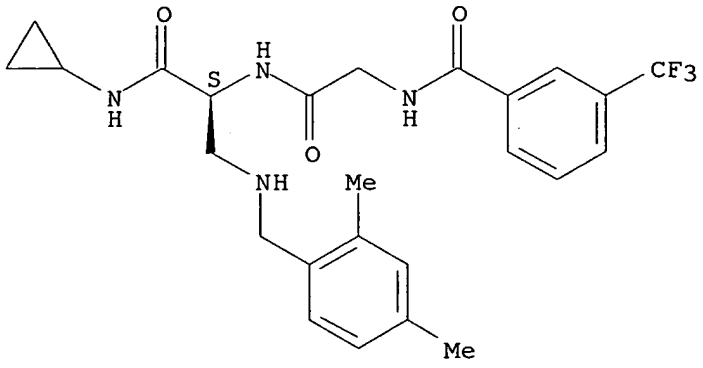
RN 439148-70-6 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



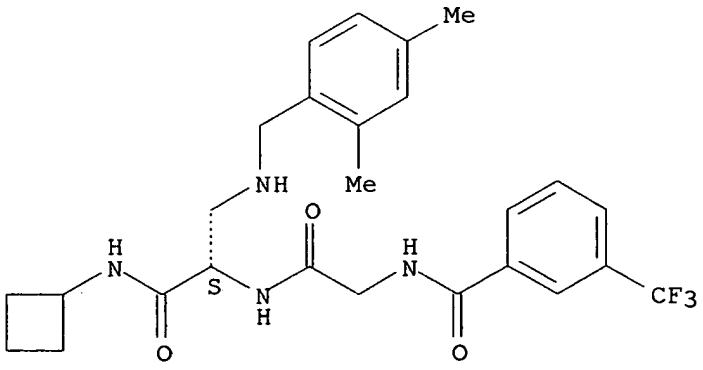
RN 439148-71-7 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclopropyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



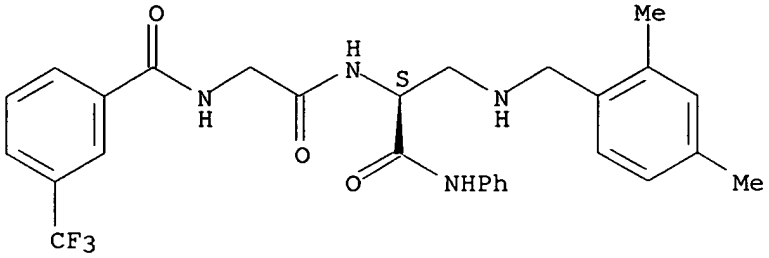
RN 439148-72-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclobutyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



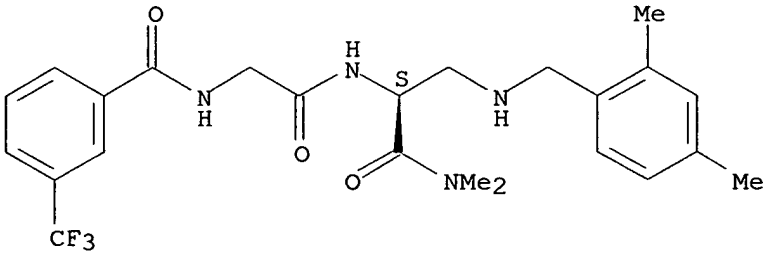
RN 439148-73-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



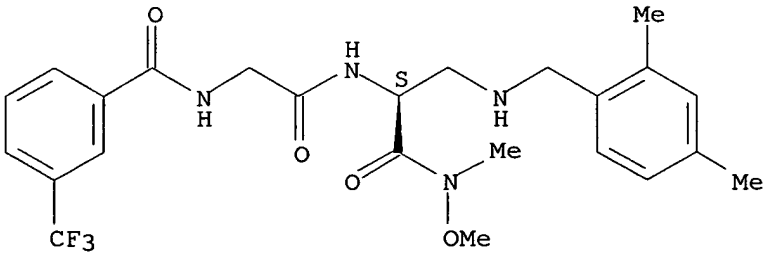
RN 439148-74-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



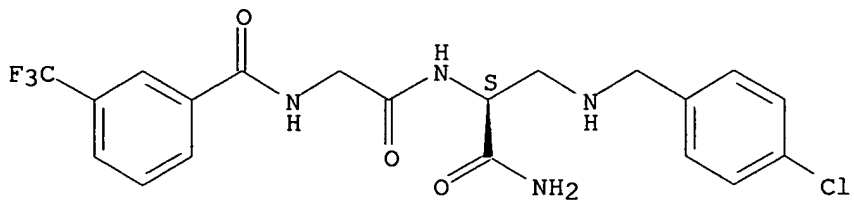
RN 439148-75-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-methoxy-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



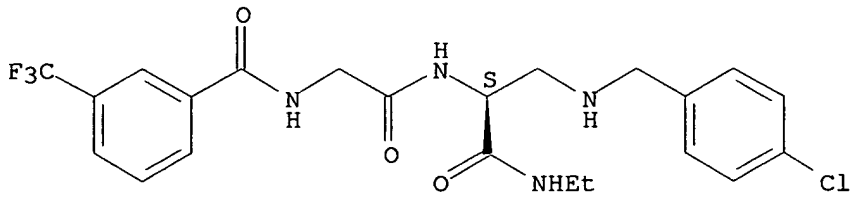
RN 439148-77-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-chlorophenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



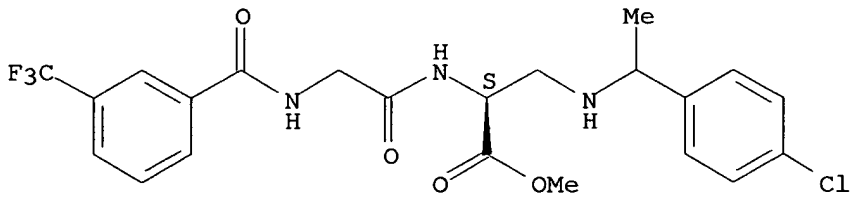
RN 439148-78-4 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-chlorophenyl)methyl]amino]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



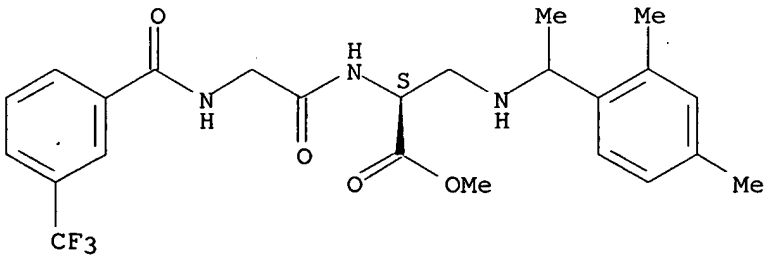
RN 439148-79-5 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[1-(4-chlorophenyl)ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439148-80-8 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[1-(2,4-dimethylphenyl)ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

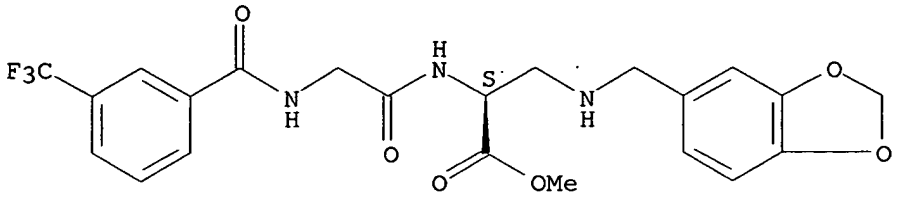
Absolute stereochemistry.



RN 439148-83-1 CAPLUS

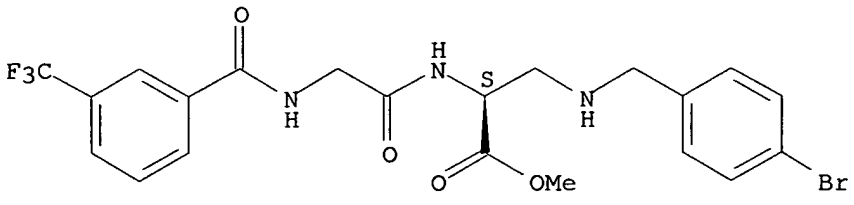
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[(1,3-benzodioxol-5-ylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



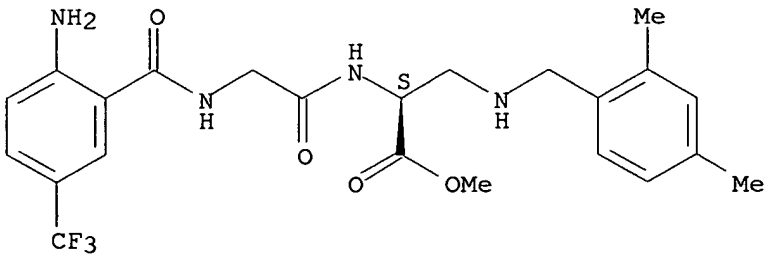
RN 439148-84-2 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromophenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



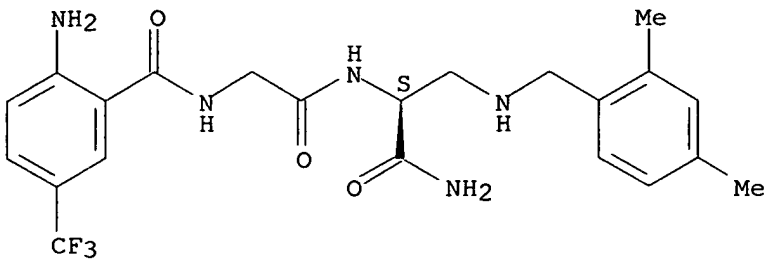
RN 439148-86-4 CAPLUS
CN L-Alanine, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



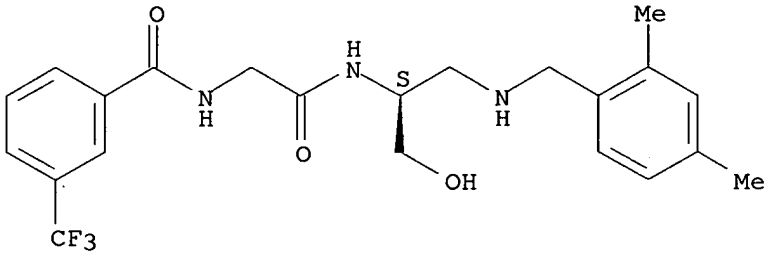
RN 439148-89-7 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



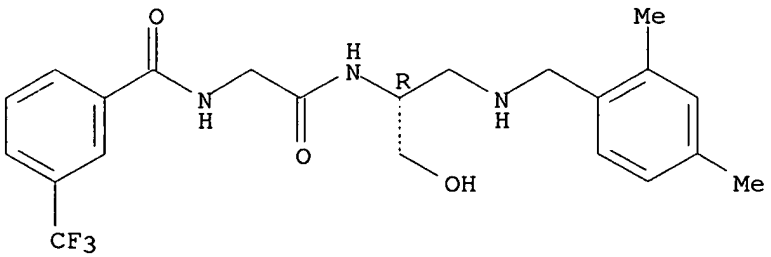
RN 439148-91-1 CAPLUS
CN Benzamide, N-[2-[[(1S)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-(hydroxymethyl)ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



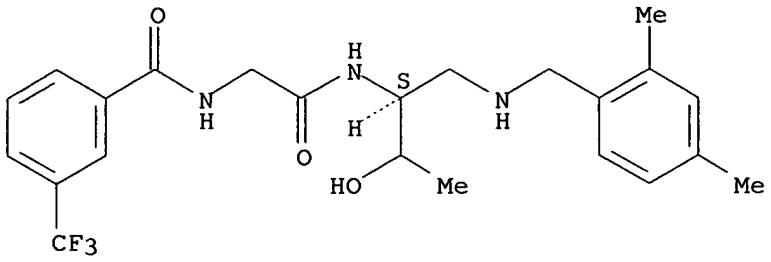
RN 439148-94-4 CAPLUS
CN Benzamide, N-[2-[[(1R)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-(hydroxymethyl)ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



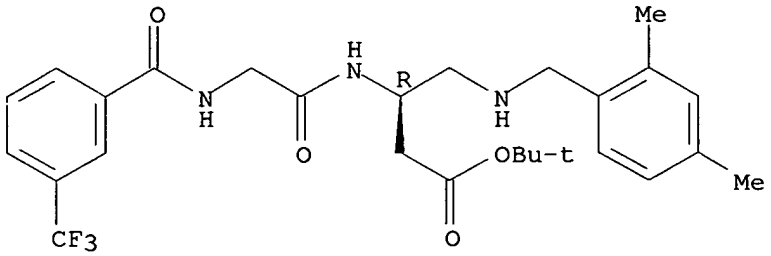
RN 439148-95-5 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



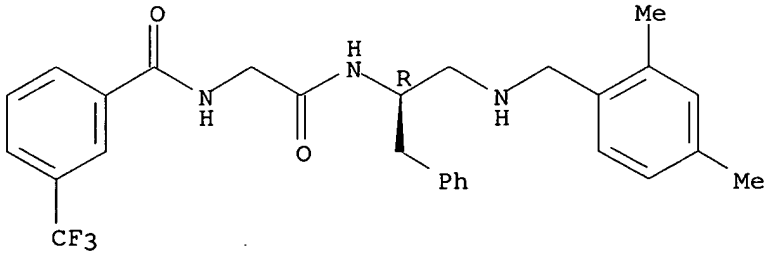
RN 439148-96-6 CAPLUS
CN Butanoic acid, 4-[[(2,4-dimethylphenyl)methyl]amino]-3-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



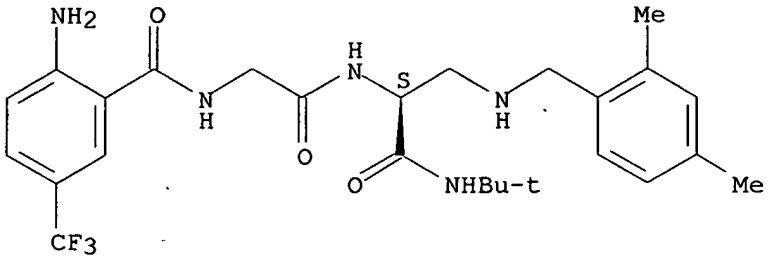
RN 439148-97-7 CAPLUS
CN Benzamide, N-[2-[[(1R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



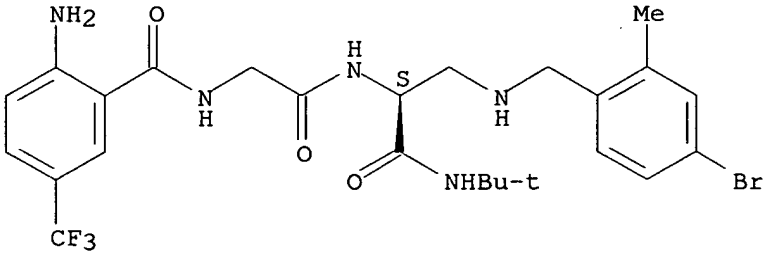
RN 439149-00-5 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



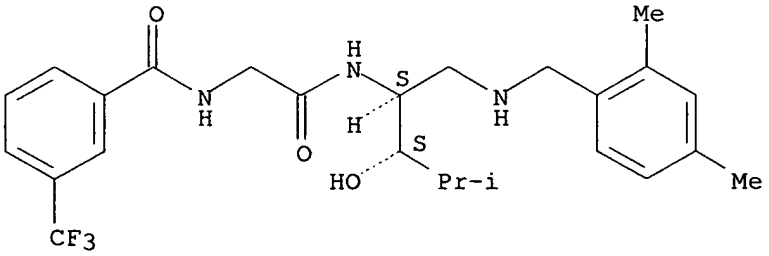
RN 439149-04-9 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



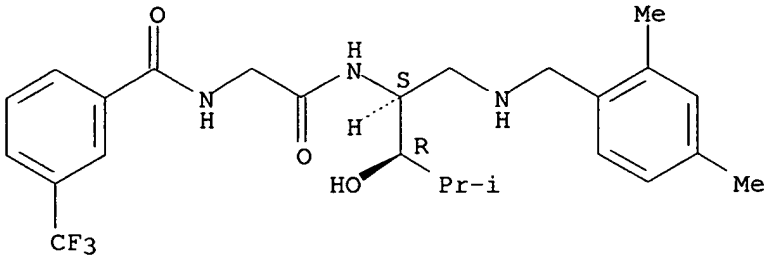
RN 439149-06-1 CAPLUS
CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



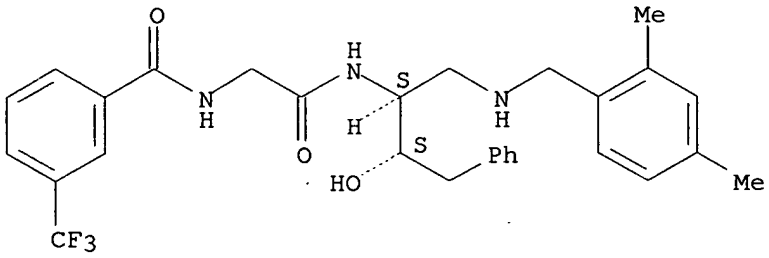
RN 439149-09-4 CAPLUS
CN D-erythro-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



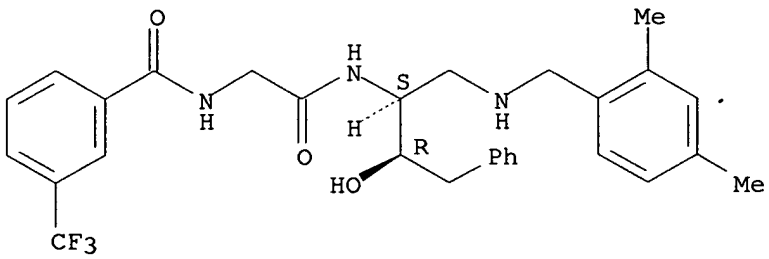
RN 439149-12-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-3-phenylpropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



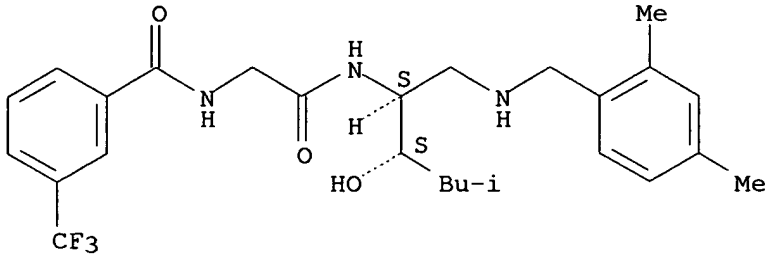
RN 439149-13-0 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-3-phenylpropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



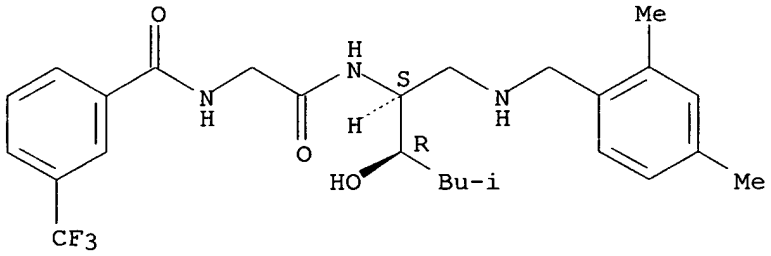
RN 439149-14-1 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



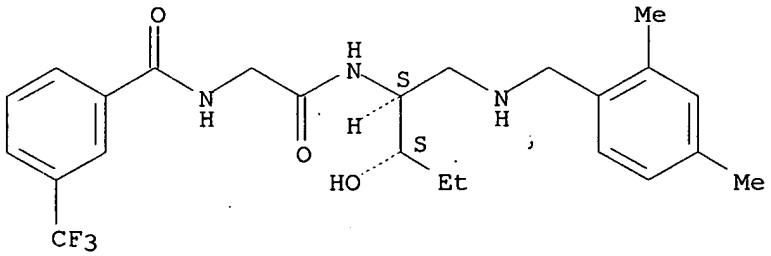
RN 439149-15-2 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



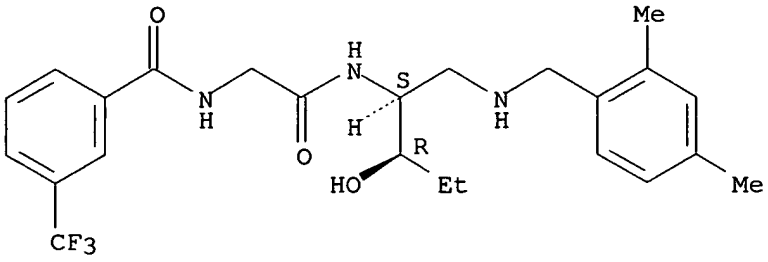
RN 439149-16-3 CAPLUS
CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



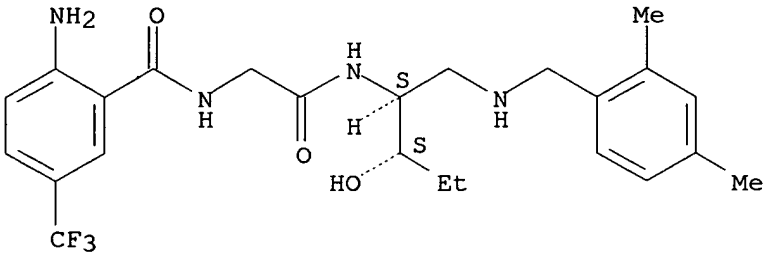
RN 439149-17-4 CAPLUS
CN D-erythro-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



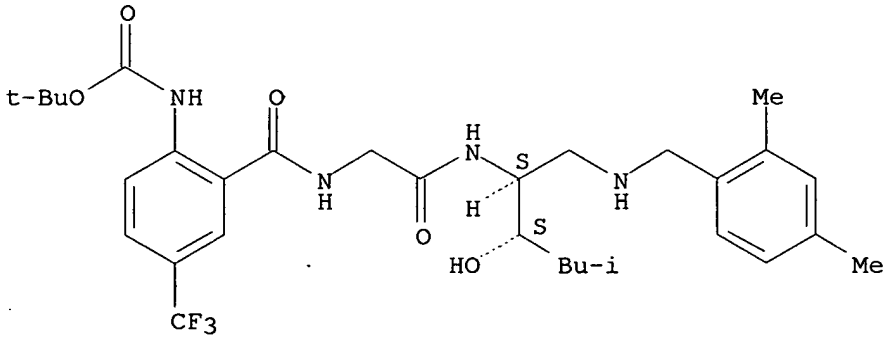
RN 439149-19-6 CAPLUS
CN D-erythro-Pentitol, 2-[[[[2-amino-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



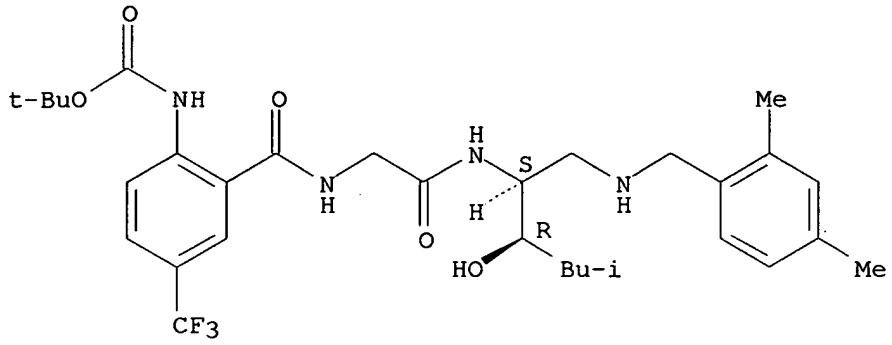
RN 439149-20-9 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



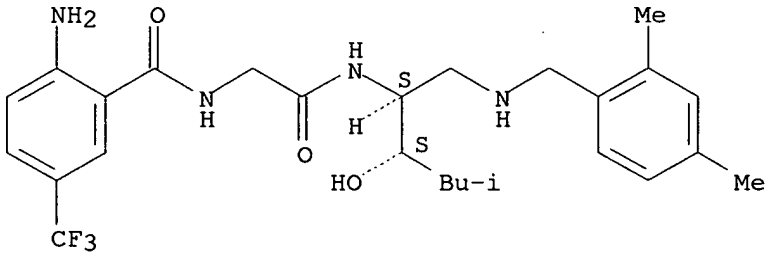
RN 439149-21-0 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



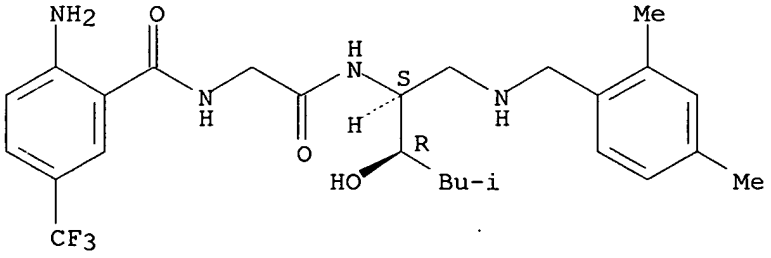
RN 439149-22-1 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



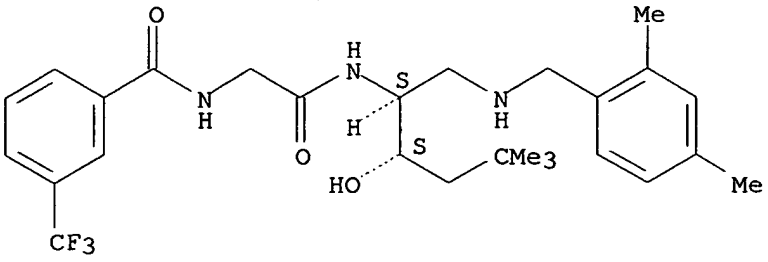
RN 439149-23-2 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



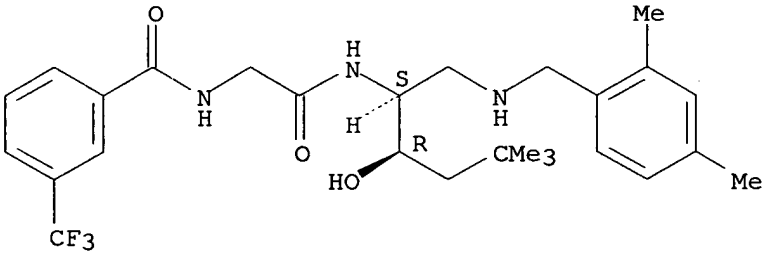
RN 439149-24-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4,4-dimethylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



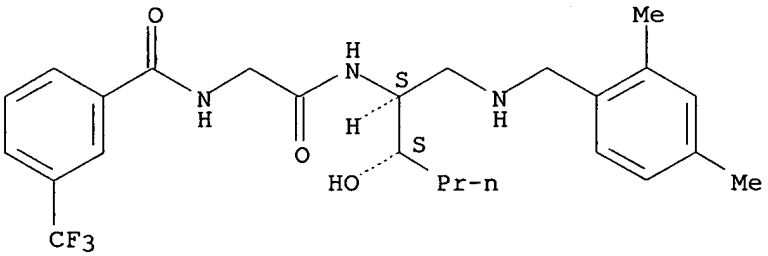
RN 439149-25-4 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4,4-dimethylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



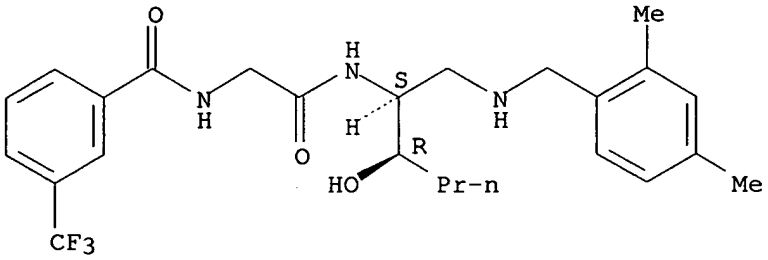
RN 439149-26-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



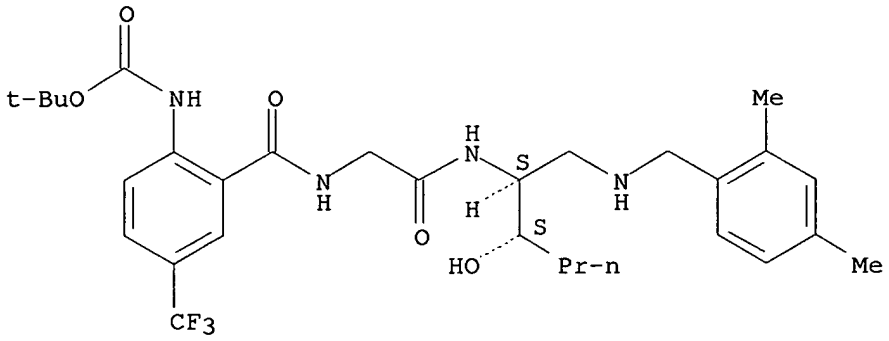
RN 439149-27-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



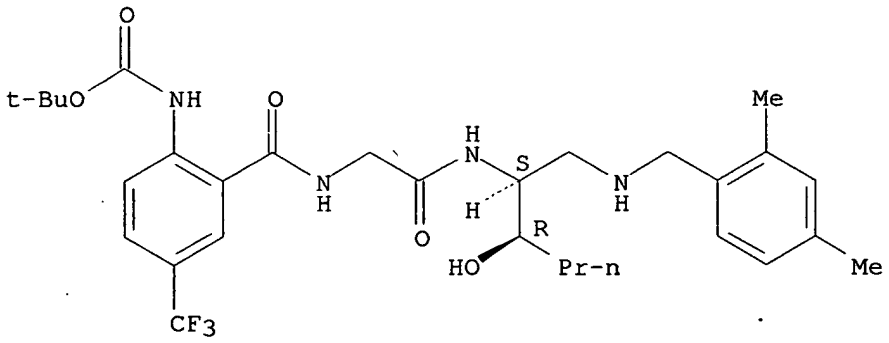
RN 439149-28-7 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



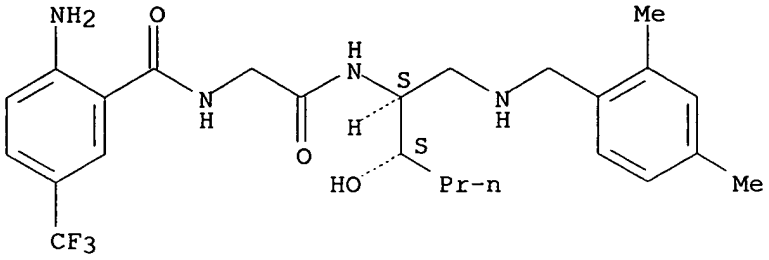
RN 439149-29-8 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



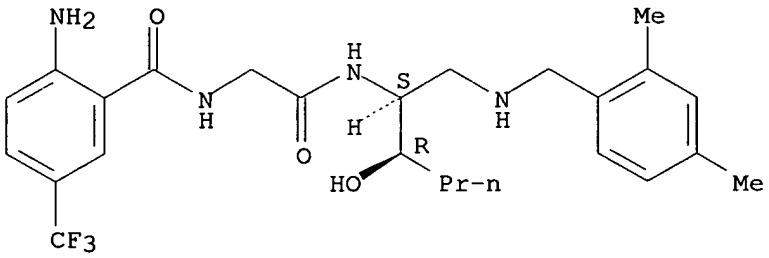
RN 439149-30-1 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



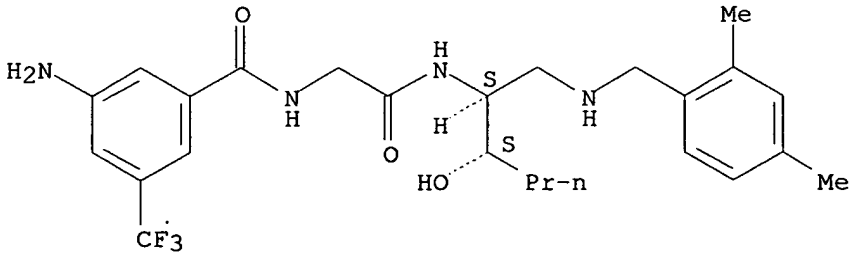
RN 439149-31-2 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



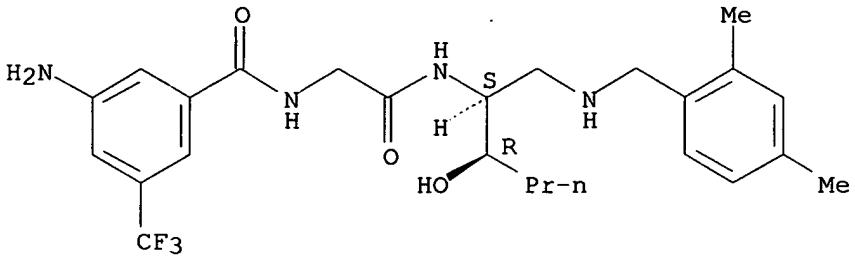
RN 439149-32-3 CAPLUS
CN Benzamide, 3-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



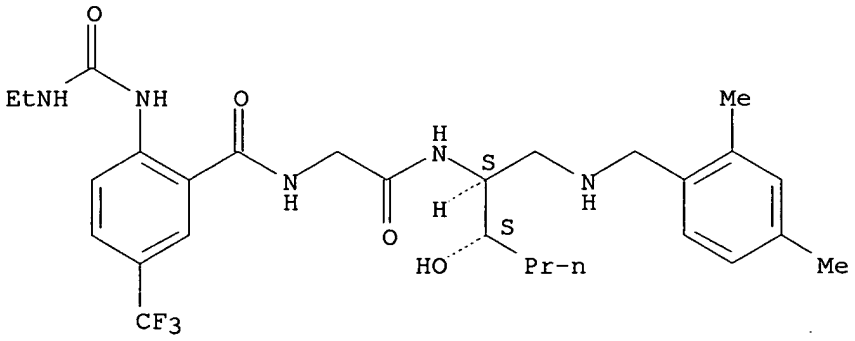
RN 439149-33-4 CAPLUS
CN Benzamide, 3-amino-N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



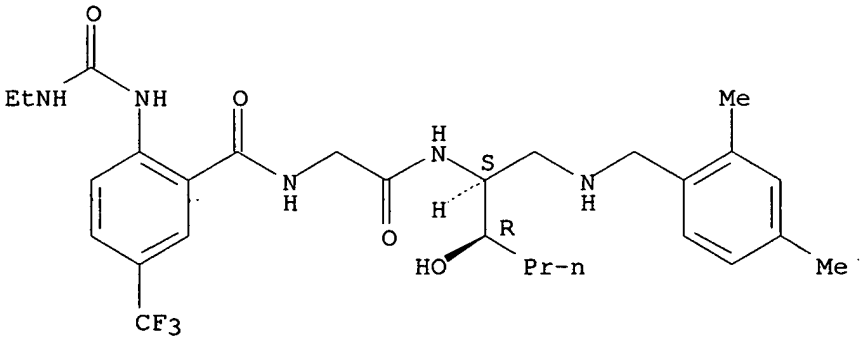
RN 439149-34-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[(ethylamino)carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



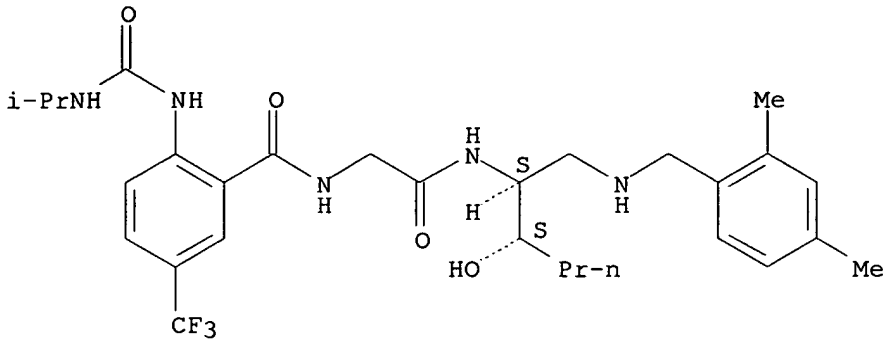
RN 439149-35-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[(ethylamino)carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



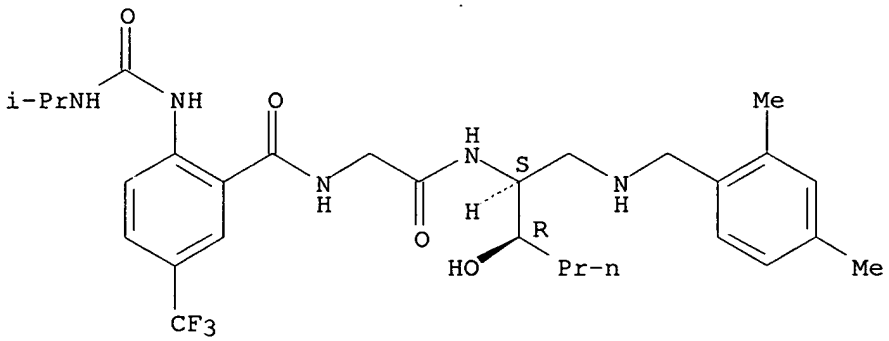
RN 439149-36-7 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



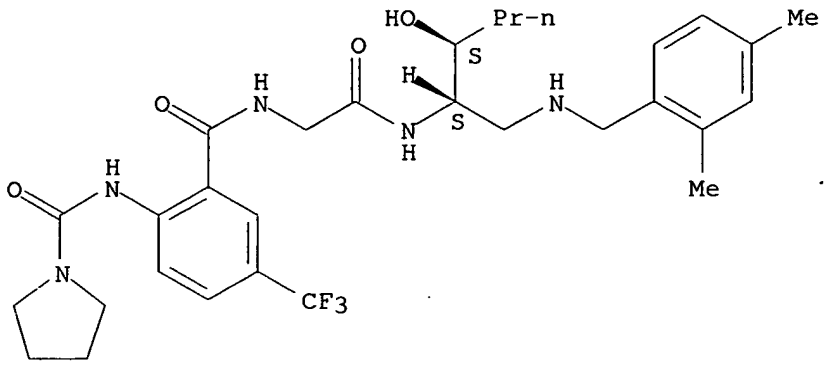
RN 439149-37-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



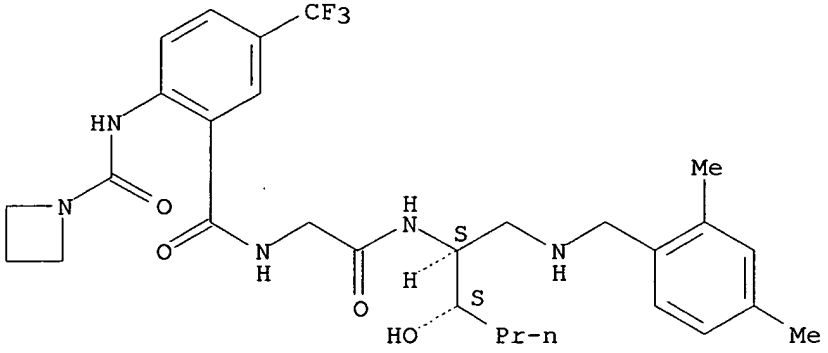
RN 439149-38-9 CAPLUS
CN 1-Pyrrolidinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



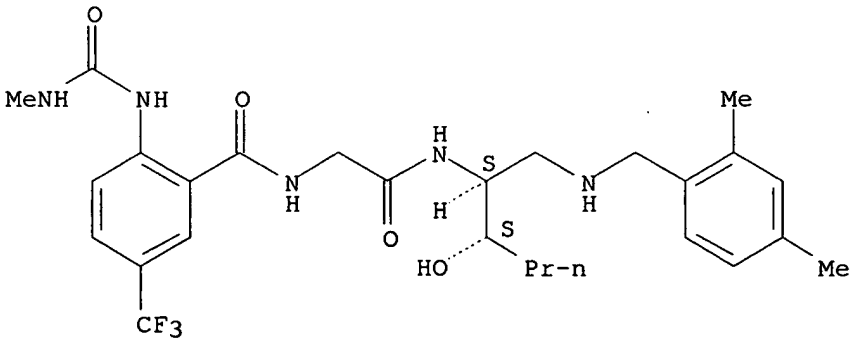
RN 439149-39-0 CAPLUS
CN 1-Azetidinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



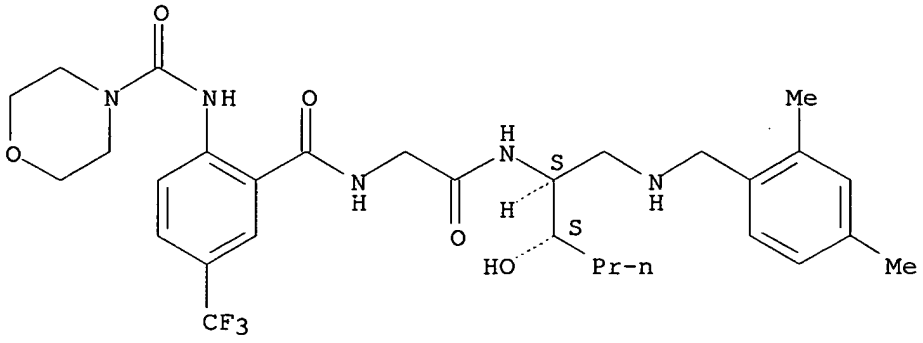
RN 439149-40-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[(methylamino)carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



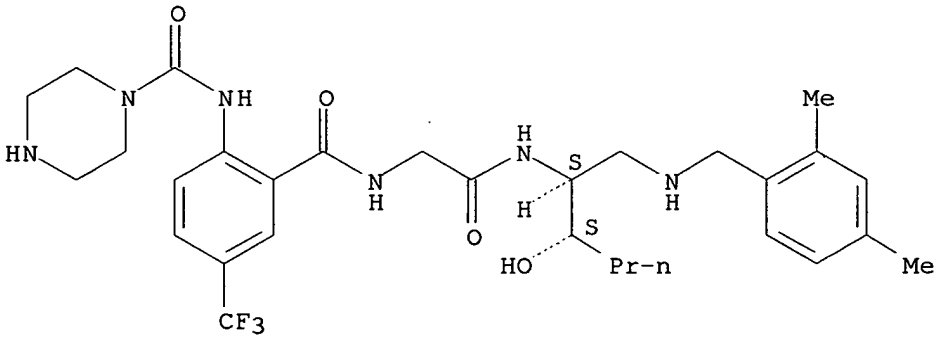
RN 439149-41-4 CAPLUS
CN 4-Morpholinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



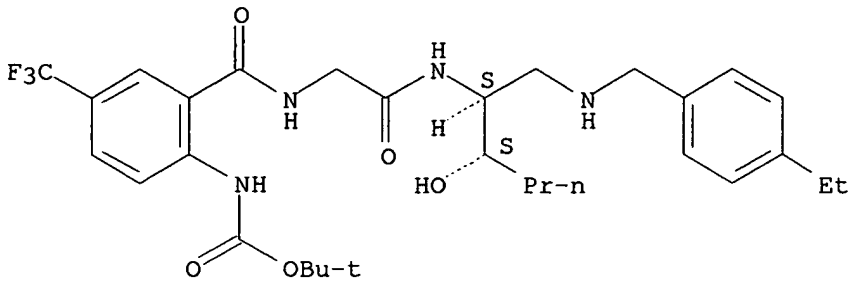
RN 439149-42-5 CAPLUS
CN 1-Piperazinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



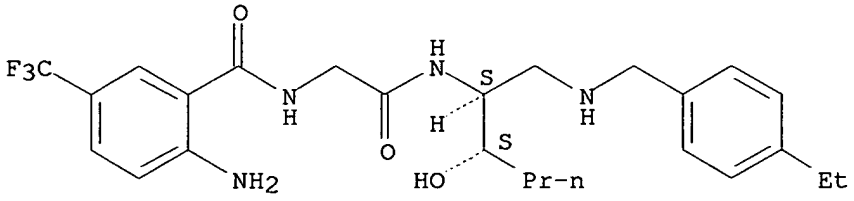
RN 439149-43-6 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



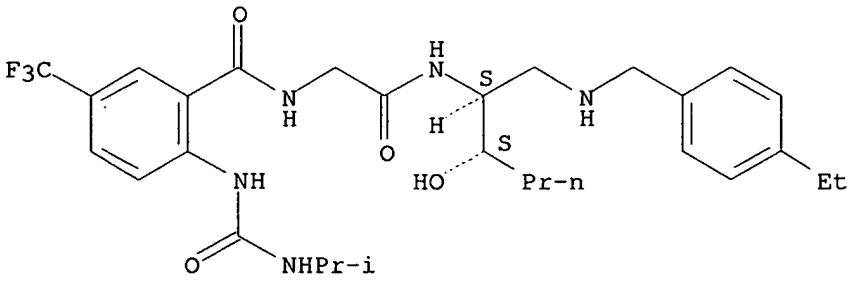
RN 439149-44-7 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



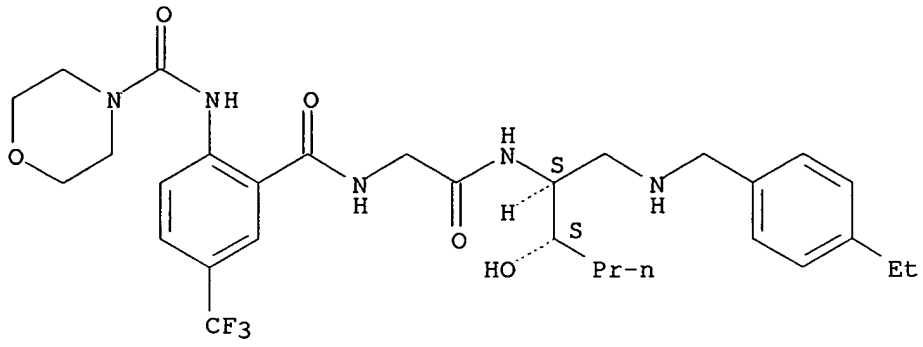
RN 439149-45-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



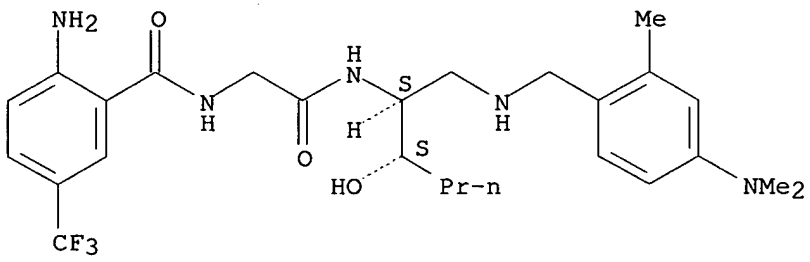
RN 439149-46-9 CAPLUS
CN 4-Morpholinecarboxamide, N-[2-[[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



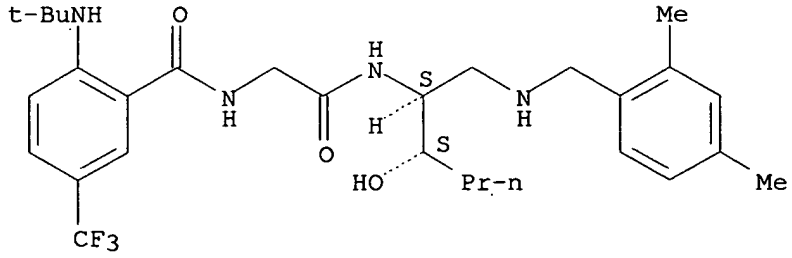
RN 439149-48-1 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[[4-(dimethylamino)-2-methylphenyl]methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



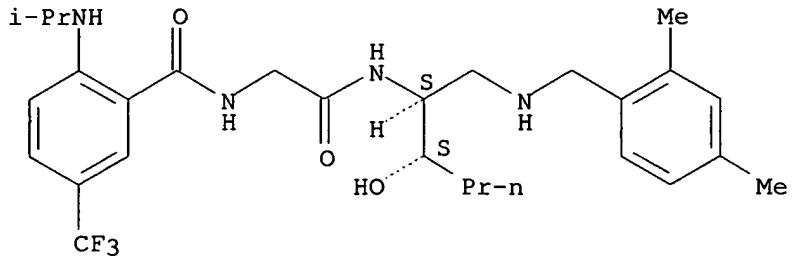
RN 439149-49-2 CAPLUS
CN Benzamide, 2-[(1,1-dimethylethyl)amino]-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



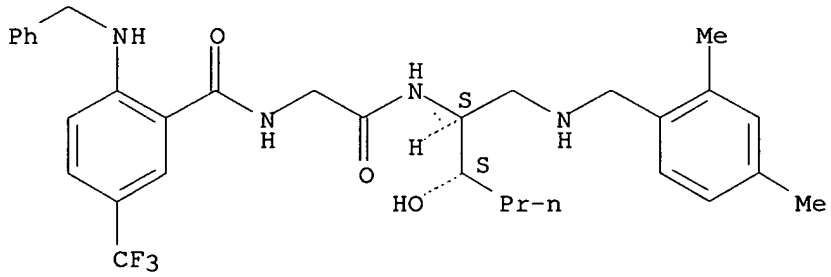
RN 439149-50-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[(1-methylethyl)amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



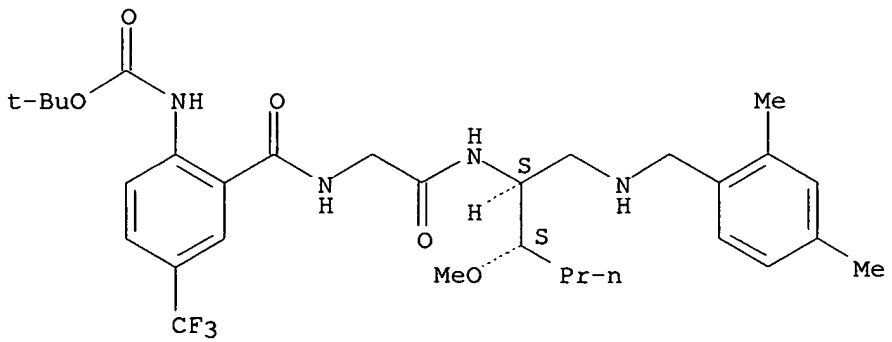
RN 439149-51-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[(phenylmethyl)amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



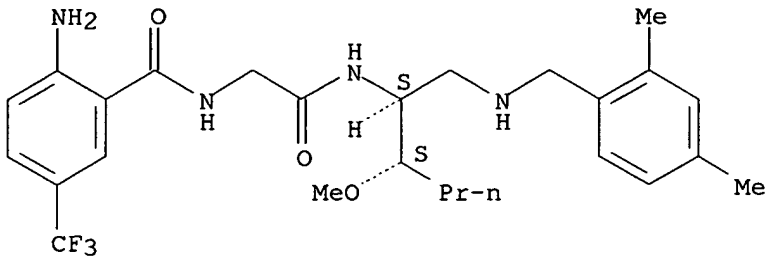
RN 439149-52-7 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-methoxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



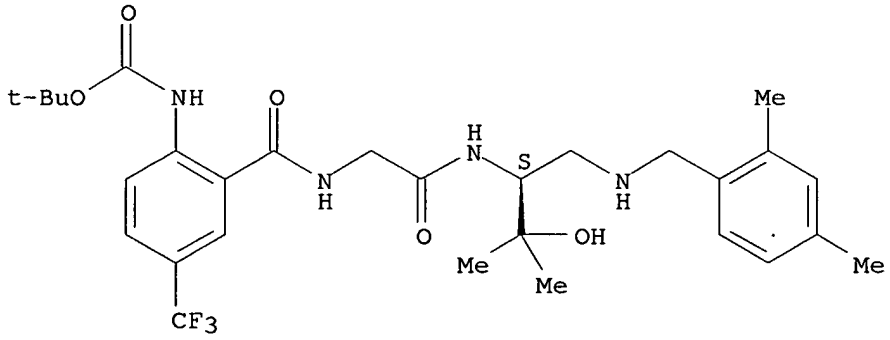
RN 439149-53-8 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-methoxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



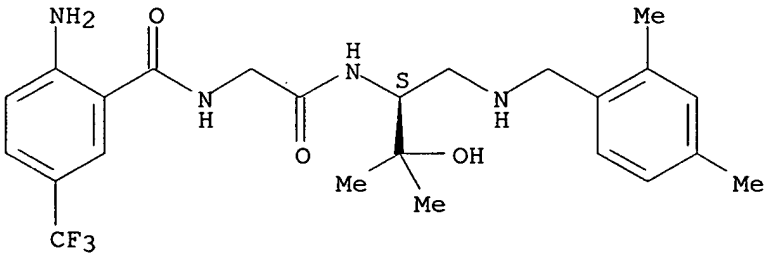
RN 439149-54-9 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-methylpropyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



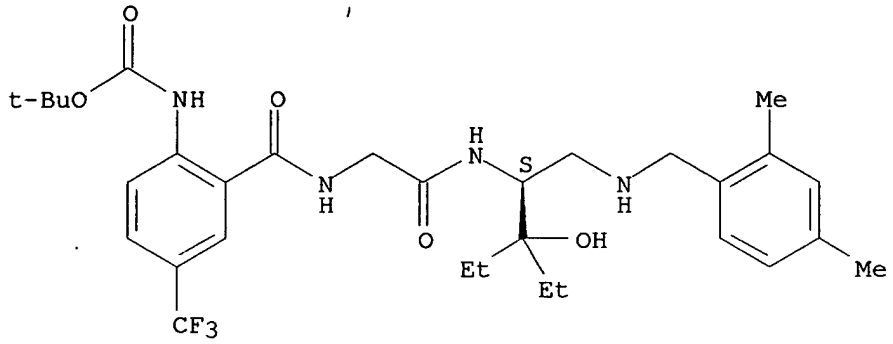
RN 439149-55-0 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-methylpropyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



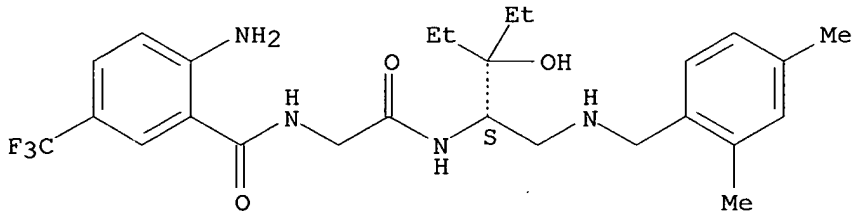
RN 439149-56-1 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-ethyl-2-hydroxybutyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



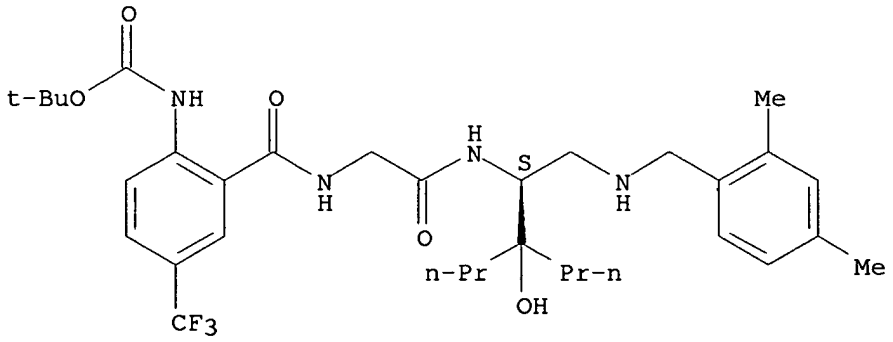
RN 439149-57-2 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-ethyl-2-hydroxybutyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



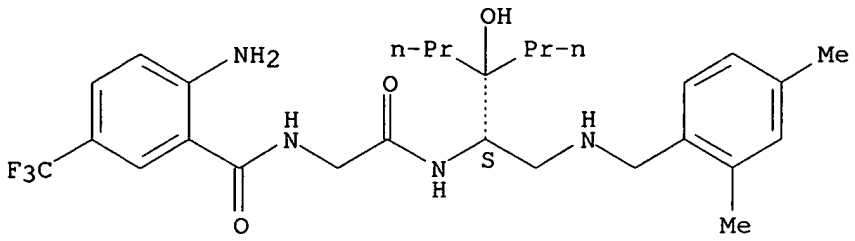
RN 439149-58-3 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-propylpentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



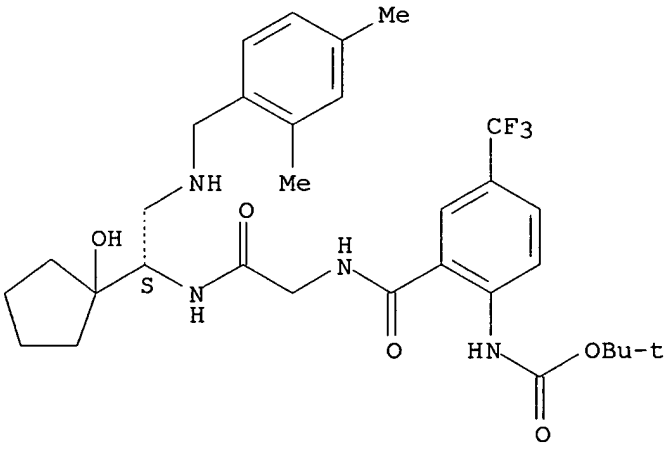
RN 439149-59-4 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-propylpentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



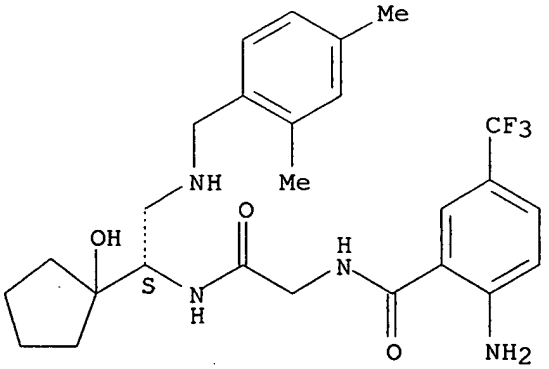
RN 439149-60-7 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-(1-hydroxycyclopentyl)ethyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



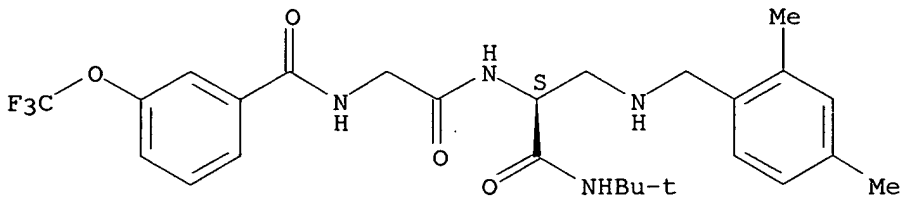
RN 439149-61-8 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-(1-hydroxycyclopentyl)ethyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



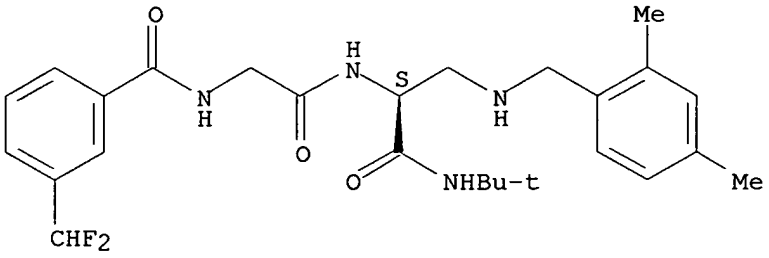
RN 439149-62-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethoxy)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



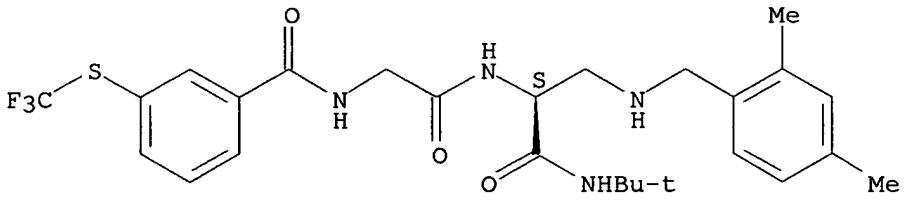
RN 439149-63-0 CAPLUS
CN L-Alaninamide, N-[3-(difluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



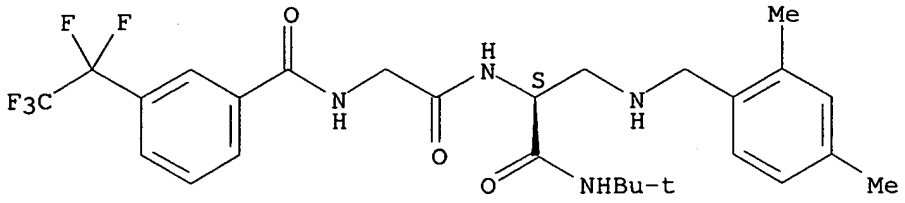
RN 439149-64-1 CAPLUS
CN L-Alaninamide, N-[3-[(trifluoromethyl)thio]benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



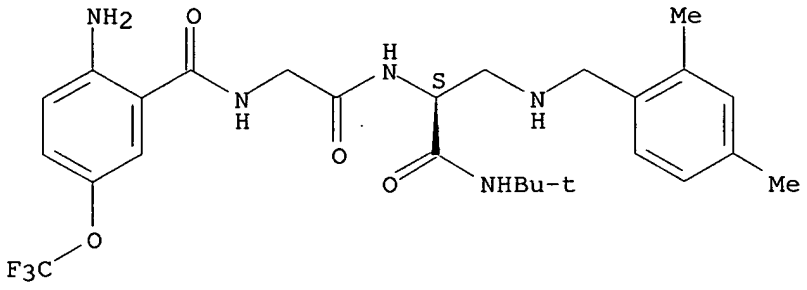
RN 439149-65-2 CAPLUS
CN L-Alaninamide, N-[3-(pentafluoroethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



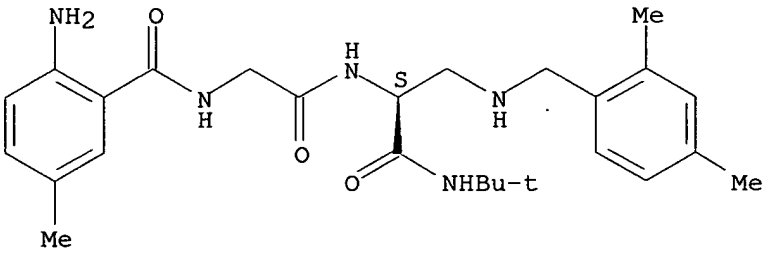
RN 439149-66-3 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethoxy)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



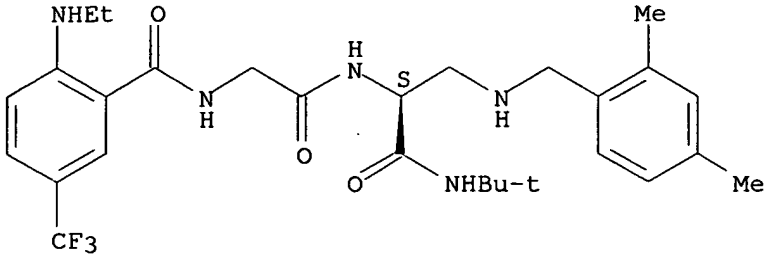
RN 439149-67-4 CAPLUS
CN L-Alaninamide, N-(2-amino-5-methylbenzoyl)glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



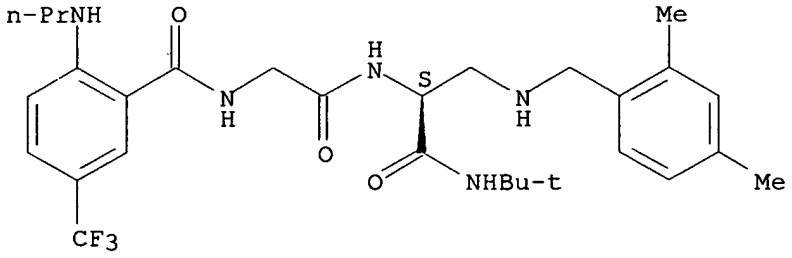
RN 439149-68-5 CAPLUS
CN L-Alaninamide, N-[2-(ethylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



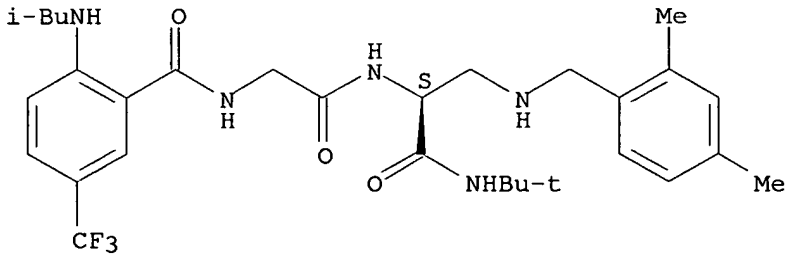
RN 439149-69-6 CAPLUS
CN L-Alaninamide, N-[2-(propylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



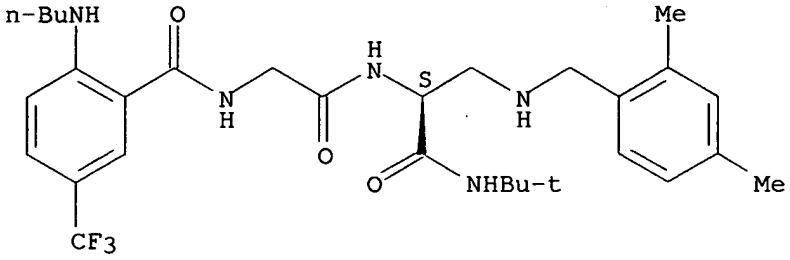
RN 439149-70-9 CAPLUS
CN L-Alaninamide, N-[2-[(2-methylpropyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



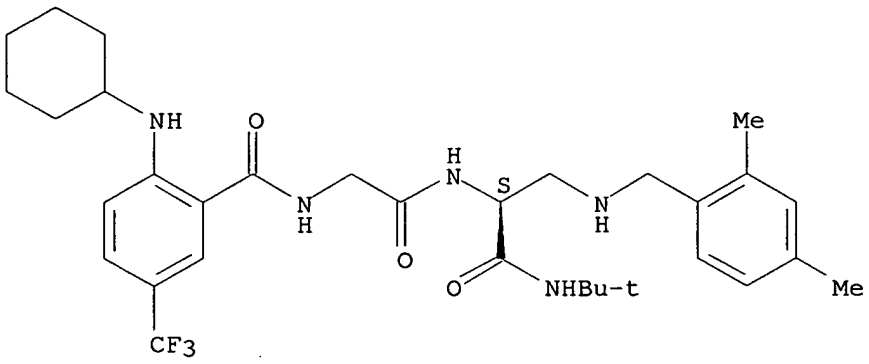
RN 439149-71-0 CAPLUS
CN L-Alaninamide, N-[2-(butylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



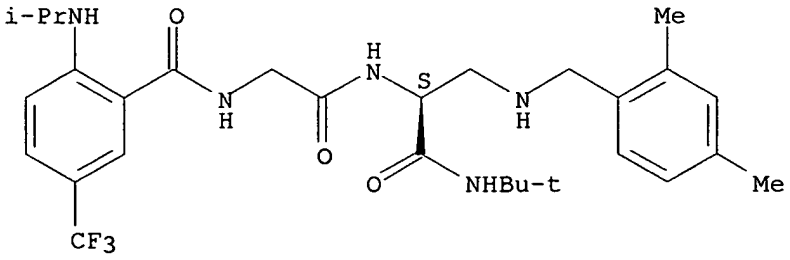
RN 439149-72-1 CAPLUS
CN L-Alaninamide, N-[2-(cyclohexylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



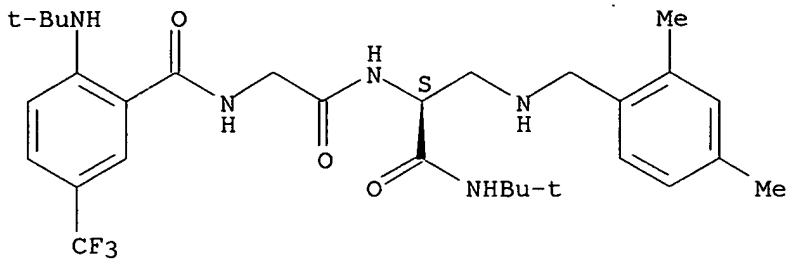
RN 439149-73-2 CAPLUS
CN L-Alaninamide, N-[2-[(1-methylethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



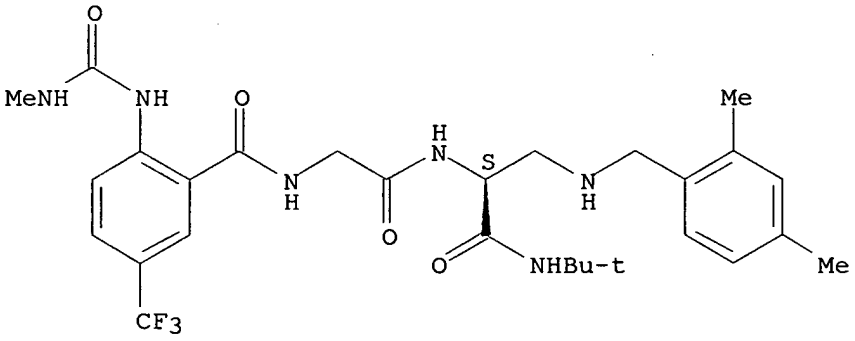
RN 439149-74-3 CAPLUS
CN L-Alaninamide, N-[2-[(1,1-dimethylethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



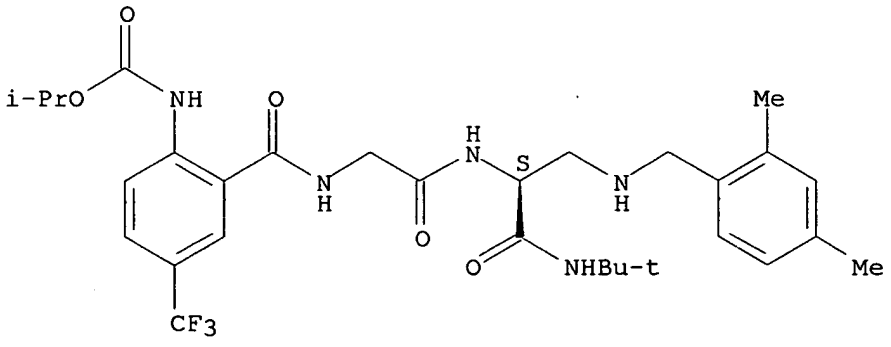
RN 439149-75-4 CAPLUS
CN L-Alaninamide, N-[2-[[(methylamino)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



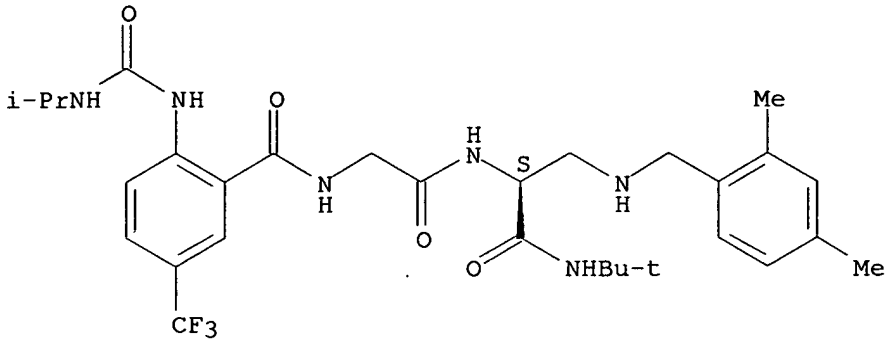
RN 439149-76-5 CAPLUS
CN L-Alaninamide, N-[2-[[(1-methylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



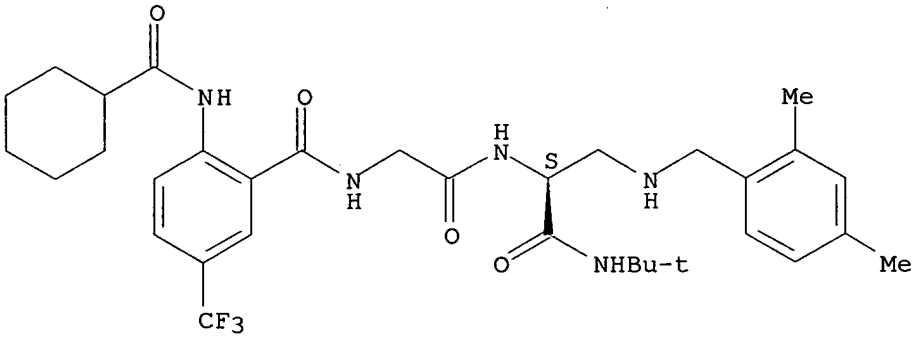
RN 439149-77-6 CAPLUS
CN L-Alaninamide, N-[2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



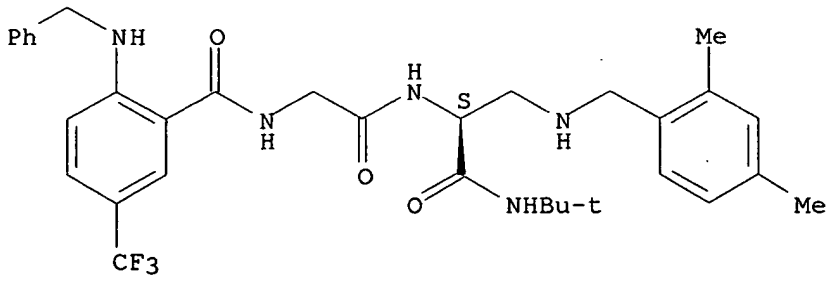
RN 439149-78-7 CAPLUS
CN L-Alaninamide, N-[2-[(cyclohexylcarbonyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439149-79-8 CAPLUS
CN L-Alaninamide, N-[2-[(phenylmethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

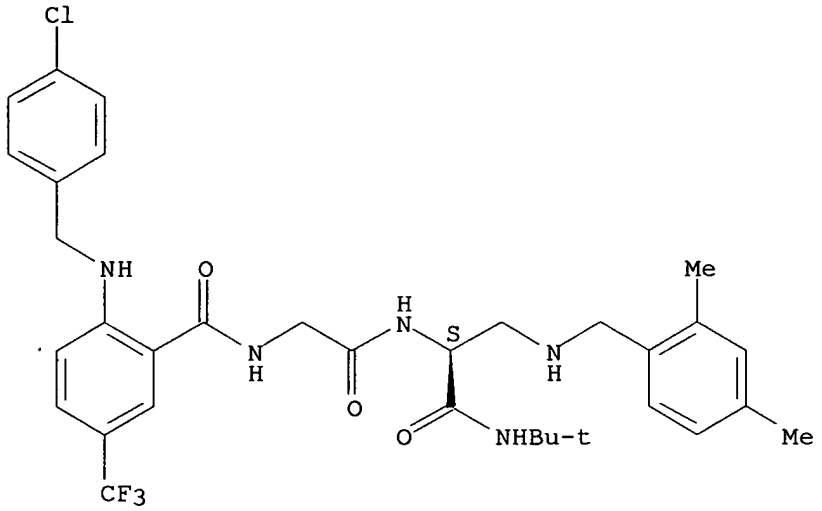
Absolute stereochemistry.



RN 439149-80-1 CAPLUS

CN L-Alaninamide, N-[2-[[(4-chlorophenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

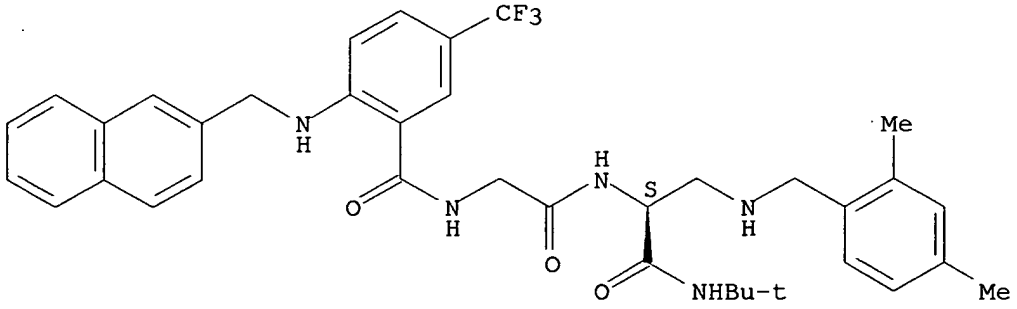
Absolute stereochemistry.



RN 439149-81-2 CAPLUS

CN L-Alaninamide, N-[2-[(2-naphthalenylmethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

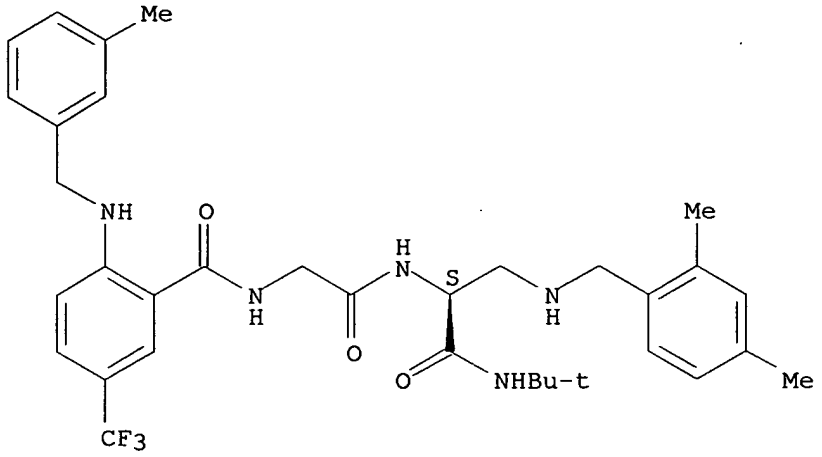
Absolute stereochemistry.



RN 439149-82-3 CAPLUS

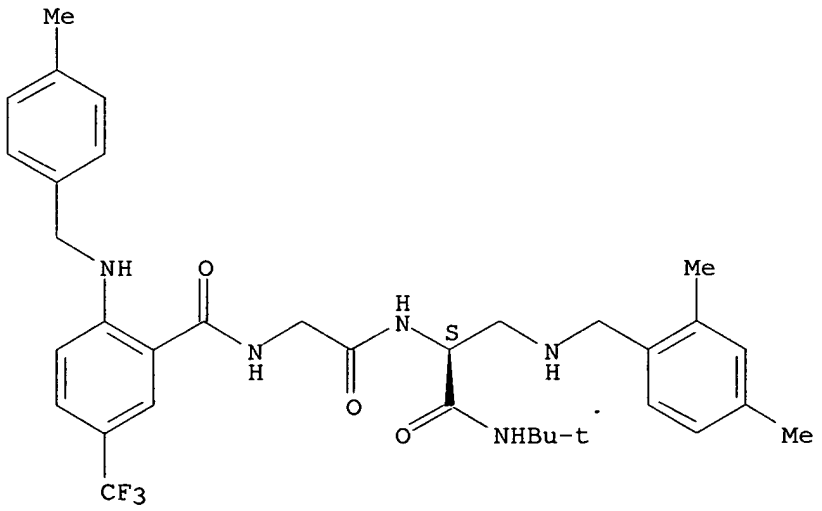
CN L-Alaninamide, N-[2-[[(3-methylphenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



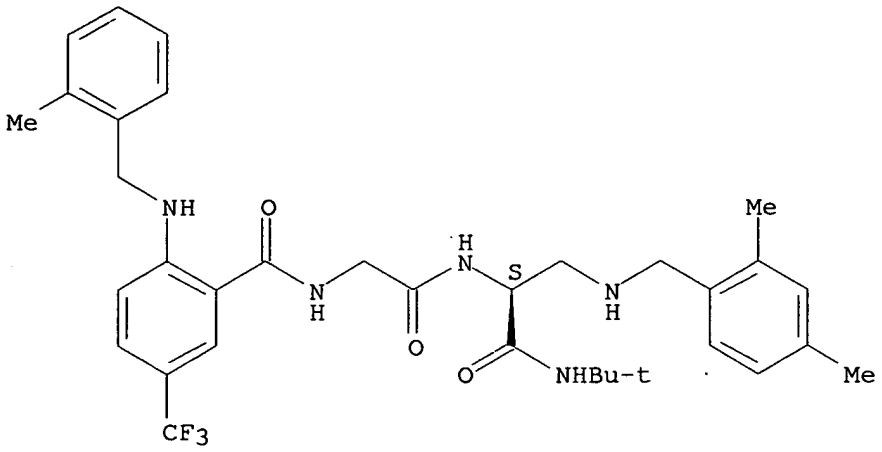
RN 439149-83-4 CAPLUS
CN L-Alaninamide, N-[2-[[(4-methylphenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



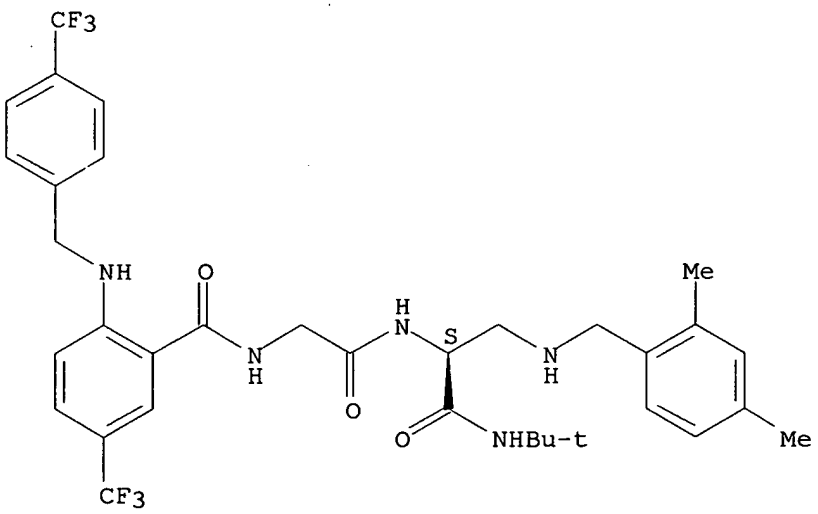
RN 439149-84-5 CAPLUS
CN L-Alaninamide, N-[2-[[(2-methylphenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



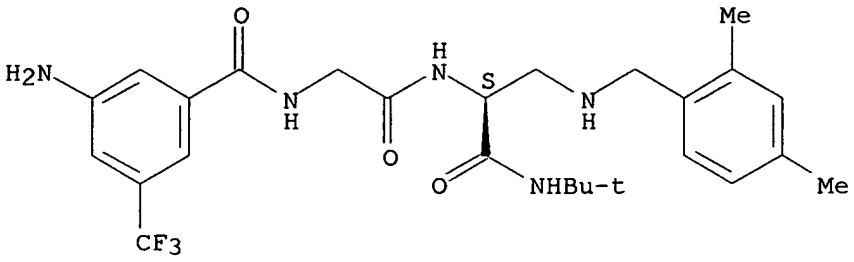
RN 439149-85-6 CAPLUS
CN L-Alaninamide, N-[5-(trifluoromethyl)-2-[[[4-(trifluoromethyl)phenyl]methyl]amino]benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



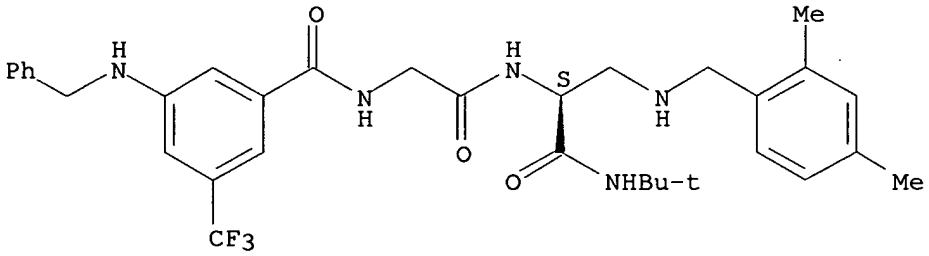
RN 439149-86-7 CAPLUS
CN L-Alaninamide, N-[3-amino-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



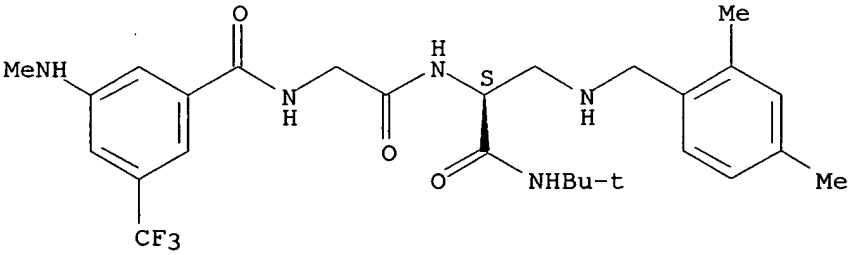
RN 439149-87-8 CAPLUS
CN L-Alaninamide, N-[3-[(phenylmethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



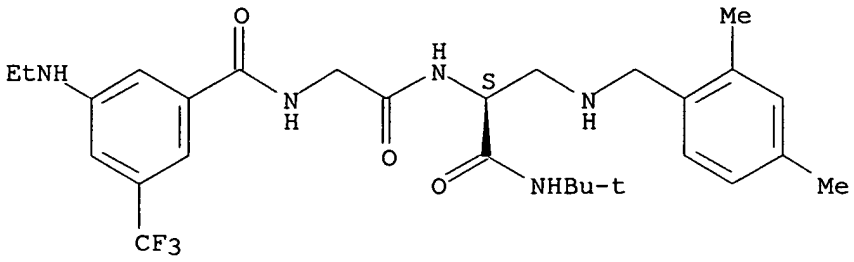
RN 439149-88-9 CAPLUS
CN L-Alaninamide, N-[3-(methylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



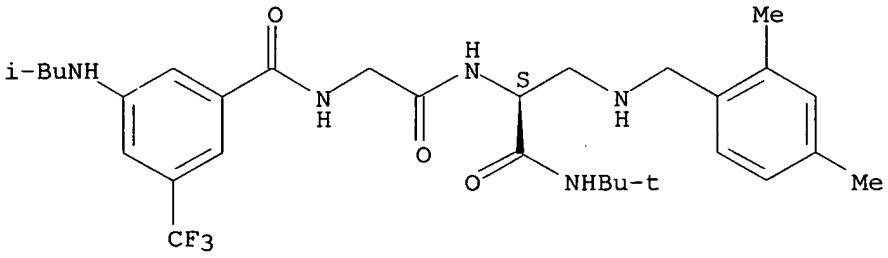
RN 439149-89-0 CAPLUS
CN L-Alaninamide, N-[3-(ethylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



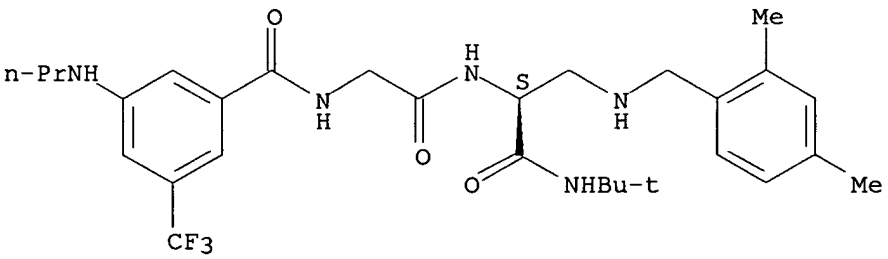
RN 439149-90-3 CAPLUS
CN L-Alaninamide, N-[3-[(2-methylpropyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



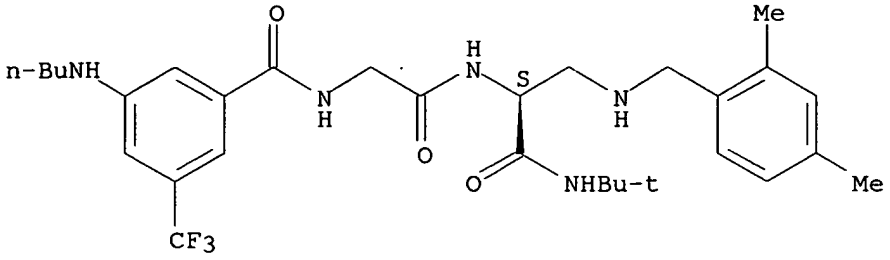
RN 439149-91-4 CAPLUS
CN L-Alaninamide, N-[3-(propylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



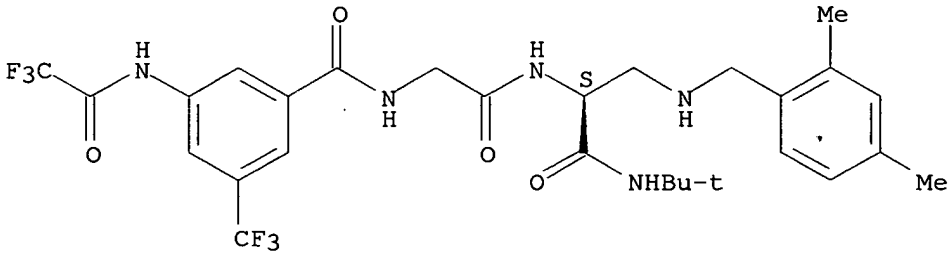
RN 439149-92-5 CAPLUS
CN L-Alaninamide, N-[3-(butylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



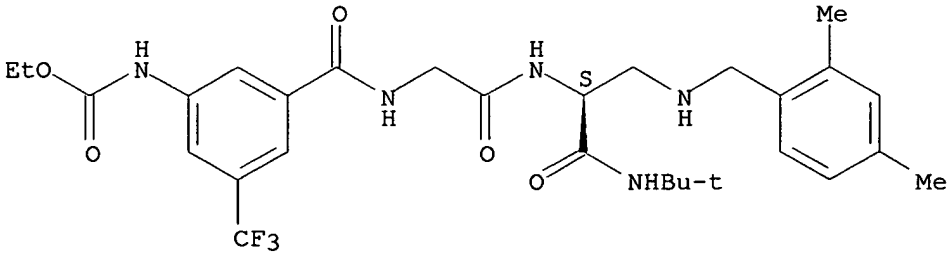
RN 439149-93-6 CAPLUS
CN L-Alaninamide, N-[3-[(trifluoroacetyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



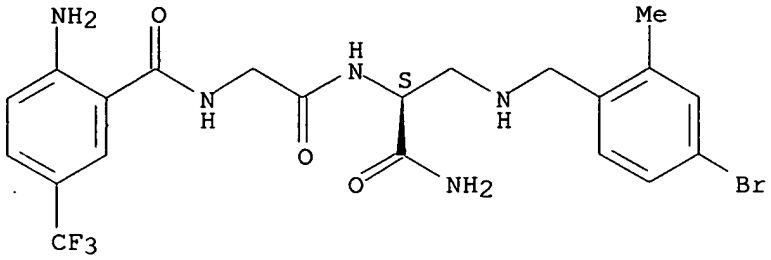
RN 439149-94-7 CAPLUS
CN L-Alaninamide, N-[3-[(ethoxycarbonyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



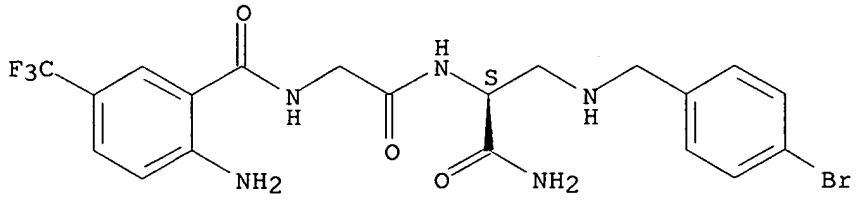
RN 439149-95-8 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



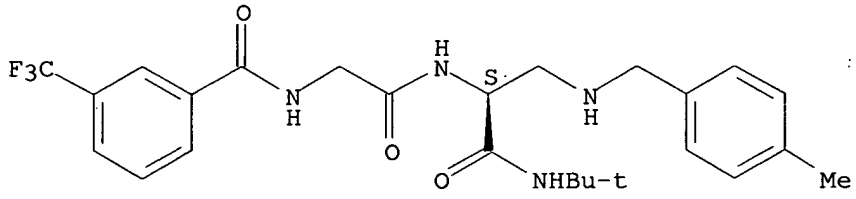
RN 439149-96-9 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromophenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



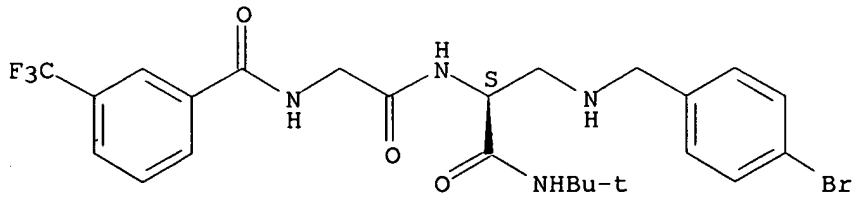
RN 439149-97-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439149-98-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromophenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

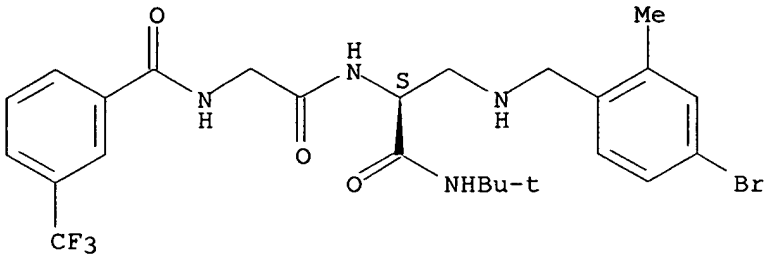
Absolute stereochemistry.



RN 439149-99-2 CAPLUS

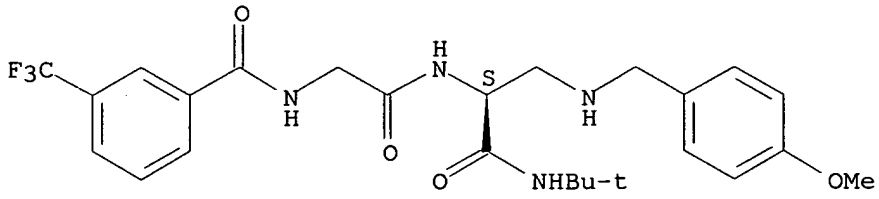
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



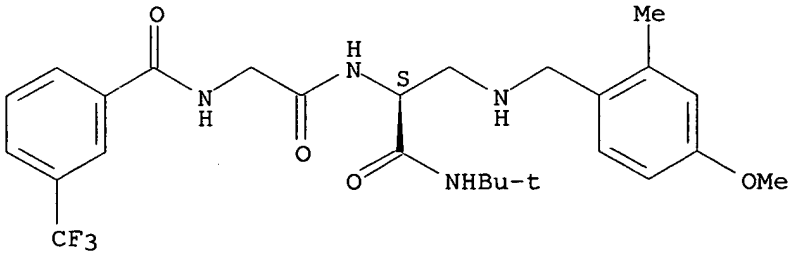
RN 439150-00-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methoxyphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



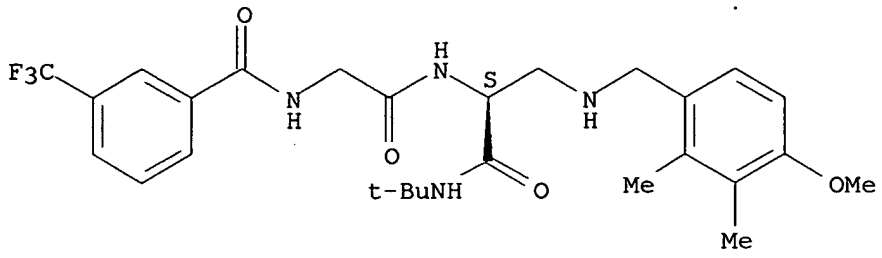
RN 439150-01-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methoxy-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



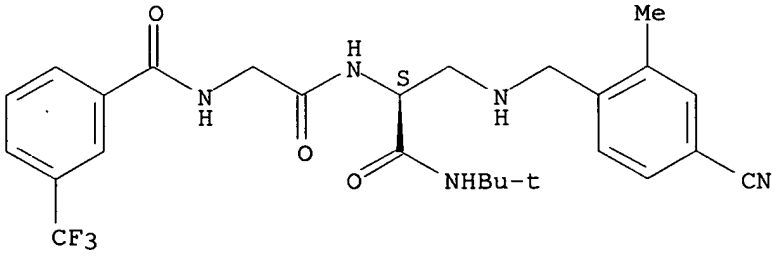
RN 439150-03-5 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methoxy-2,3-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



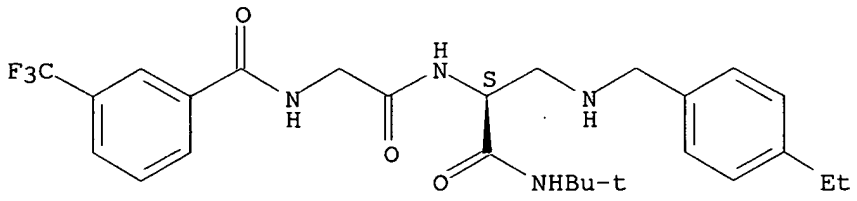
RN 439150-04-6 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-cyano-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



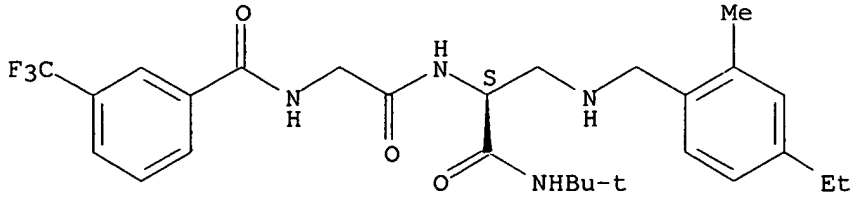
RN 439150-05-7 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-ethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



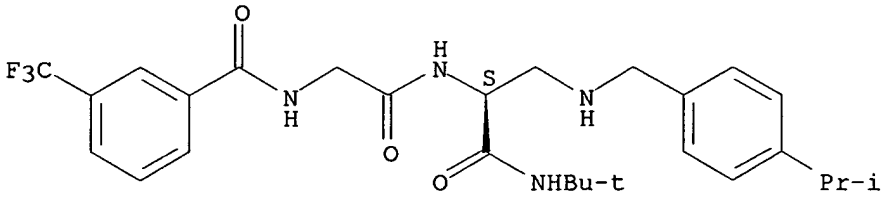
RN 439150-07-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-ethyl-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



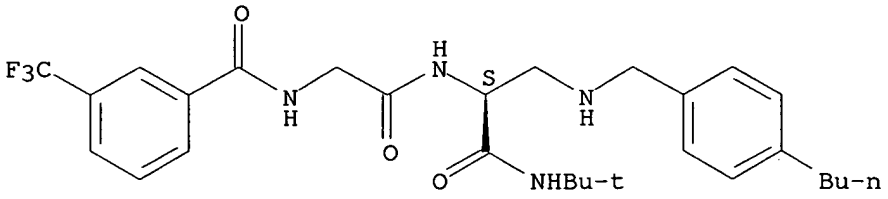
RN 439150-08-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(1-methylethyl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



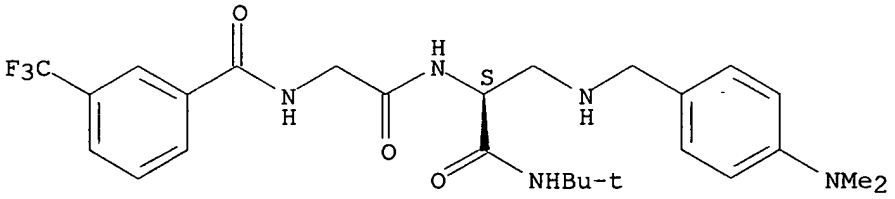
RN 439150-09-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-butylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



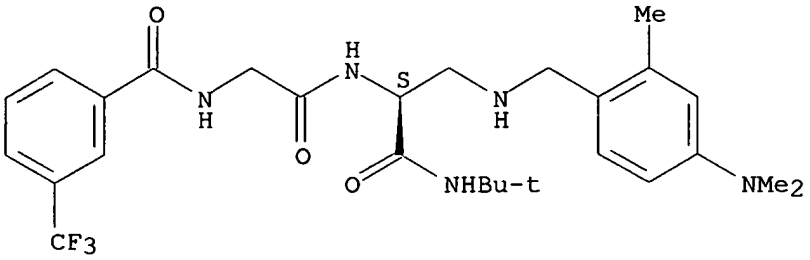
RN 439150-10-4 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[[4-(dimethylamino)phenyl]methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



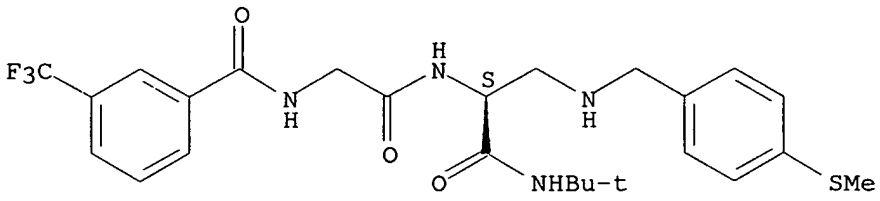
RN 439150-11-5 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[[4-(dimethylamino)-2-methylphenyl]methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



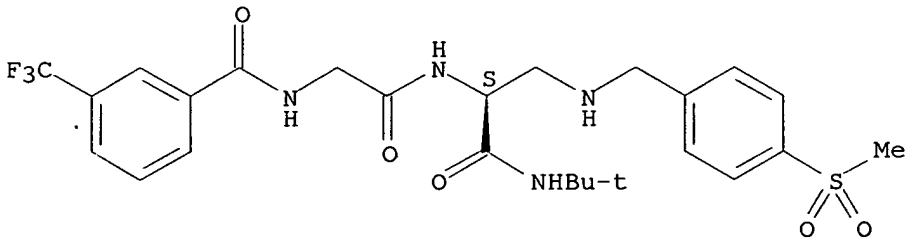
RN 439150-12-6 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(methylthio)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



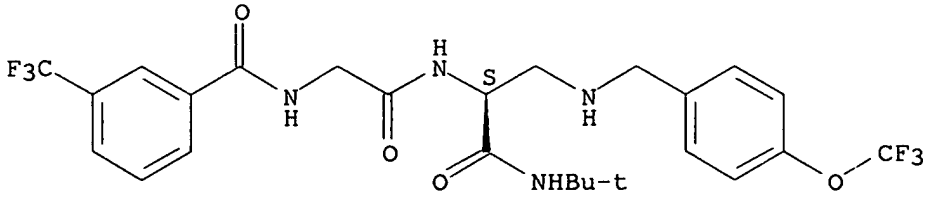
RN 439150-13-7 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(methylsulfonyl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



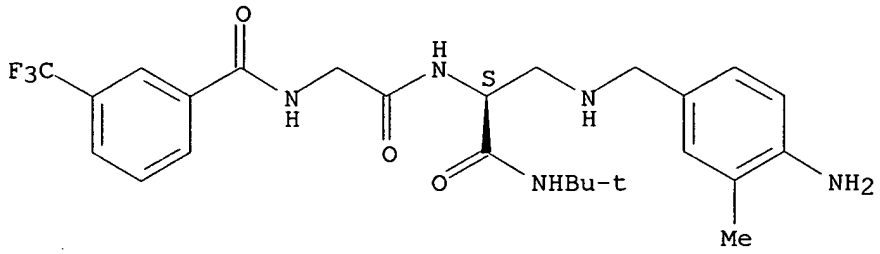
RN 439150-14-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(trifluoromethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



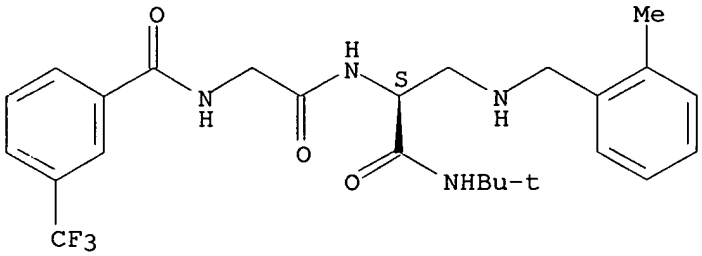
RN 439150-15-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-amino-3-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



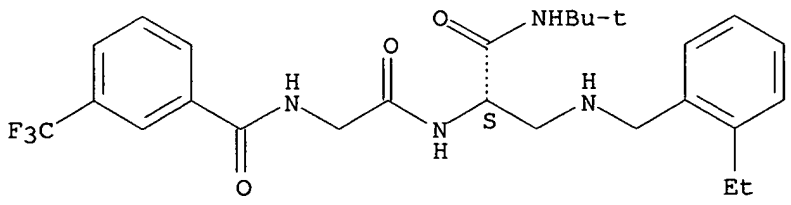
RN 439150-17-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



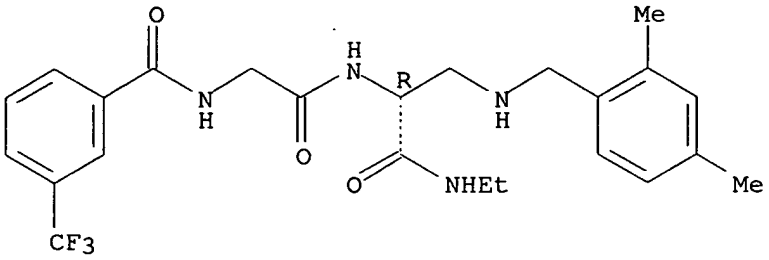
RN 439150-18-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2-ethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



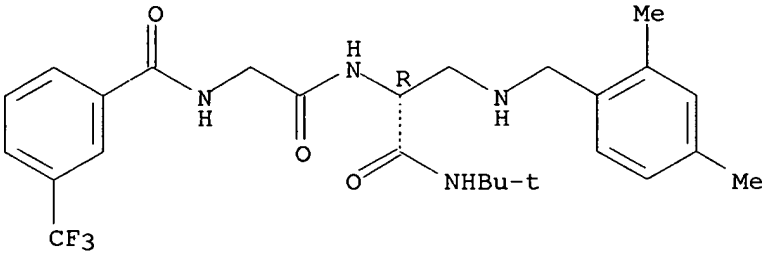
RN 439150-19-3 CAPLUS
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



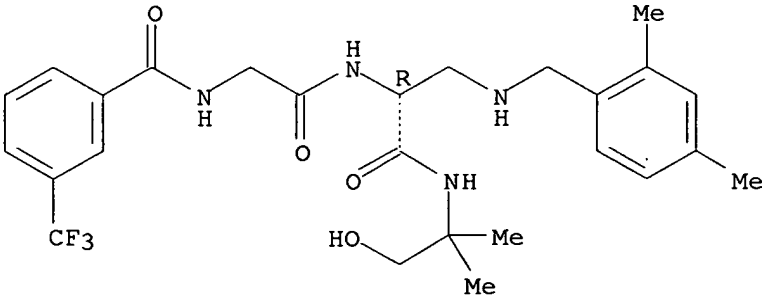
RN 439150-20-6 CAPLUS
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



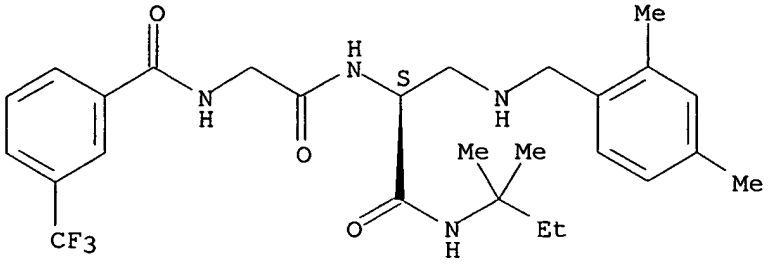
RN 439150-21-7 CAPLUS
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2-hydroxy-1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



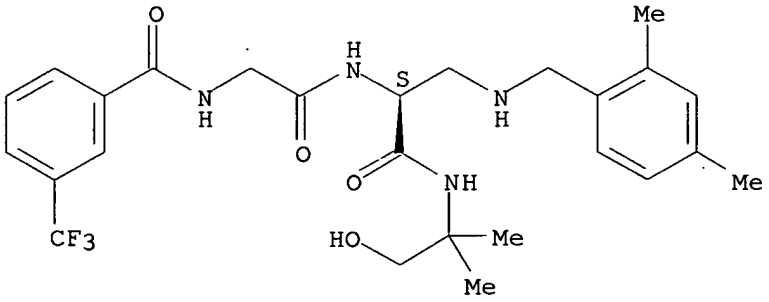
RN 439150-22-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1,1-dimethylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



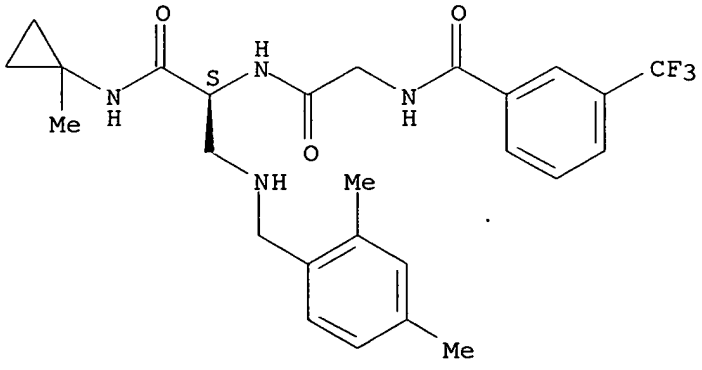
RN 439150-23-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2-hydroxy-1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



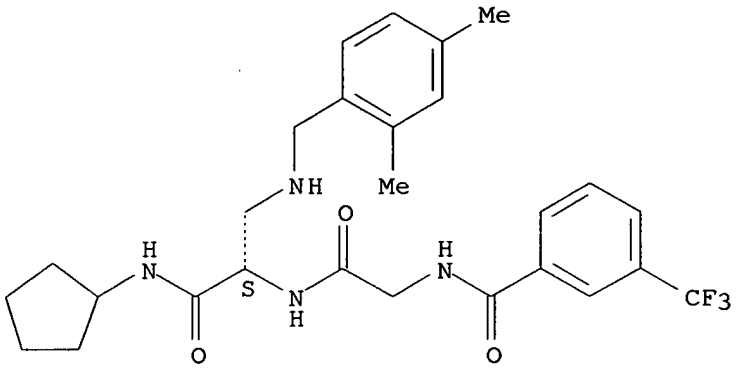
RN 439150-24-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1-methylcyclopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



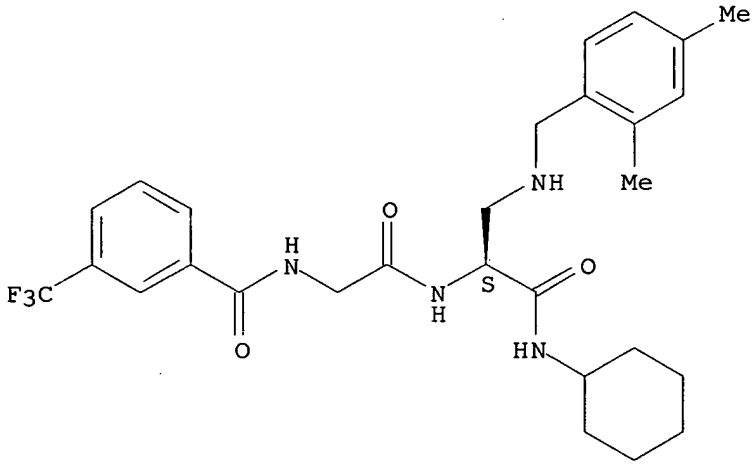
RN 439150-25-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclopentyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



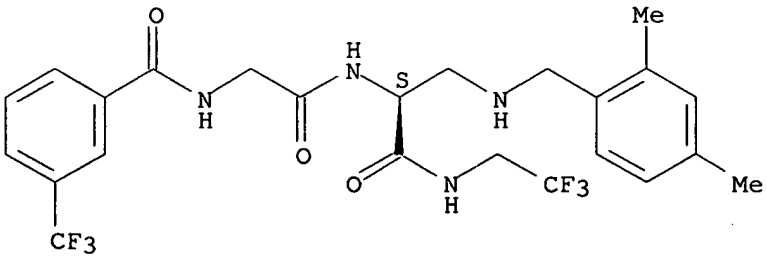
RN 439150-26-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclohexyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



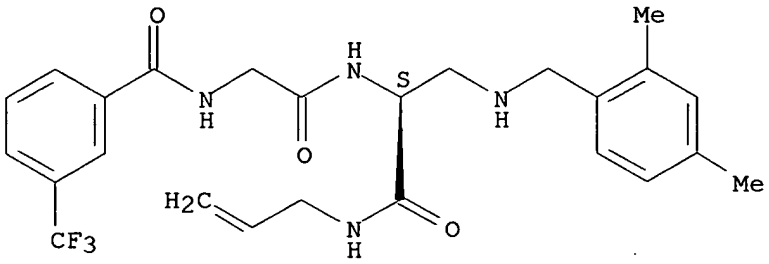
RN 439150-27-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



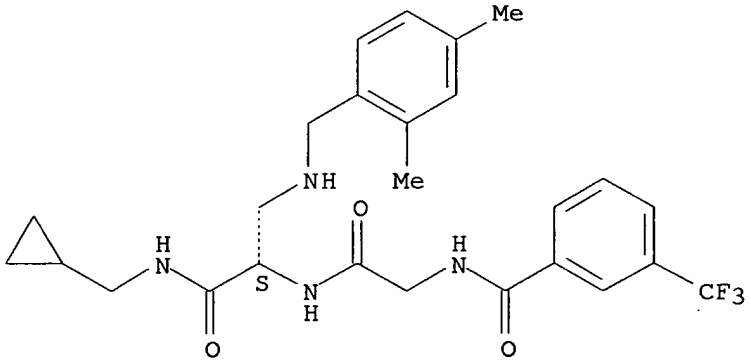
RN 439150-28-4 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



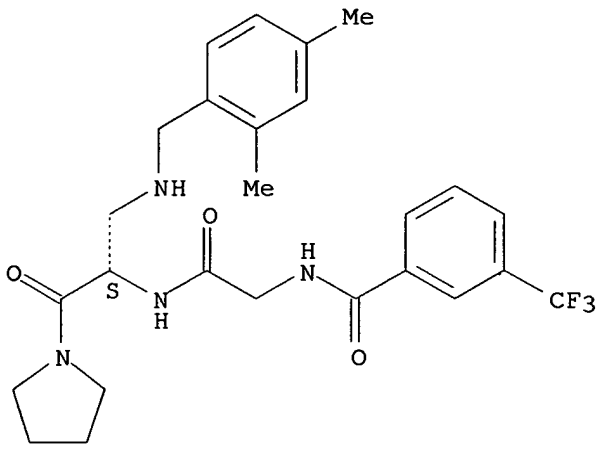
RN 439150-29-5 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(cyclopropylmethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



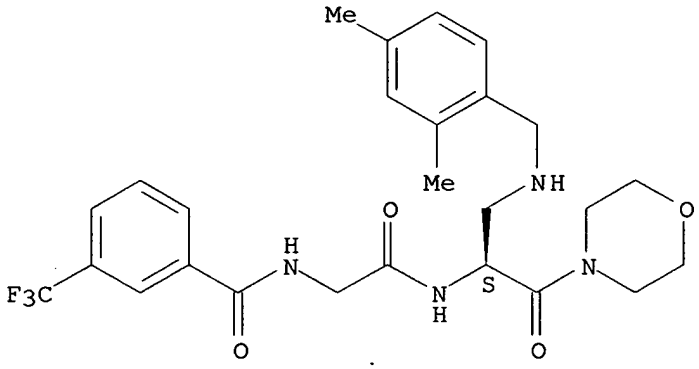
RN 439150-31-9 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-oxo-2-(1-pyrrolidinyl)ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



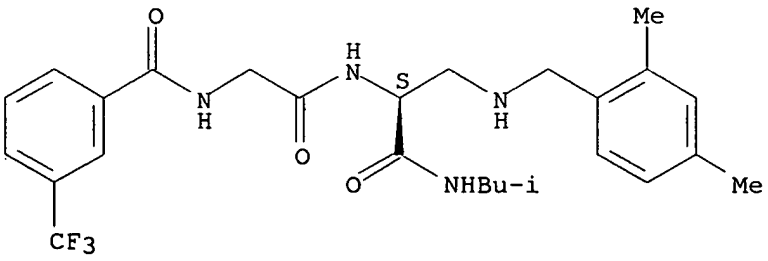
RN 439150-32-0 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-(4-morpholinyl)-2-oxoethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439150-33-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

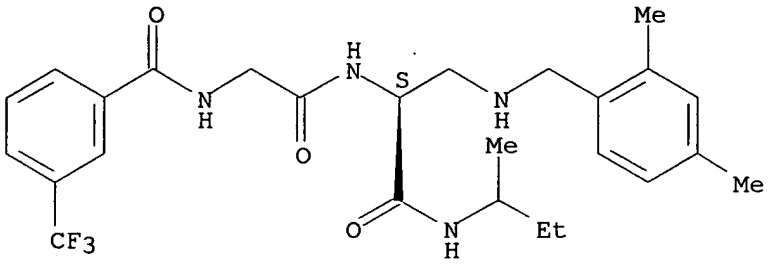
Absolute stereochemistry.



RN 439150-34-2 CAPLUS

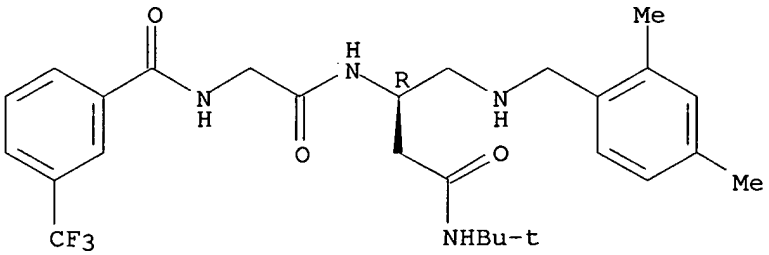
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



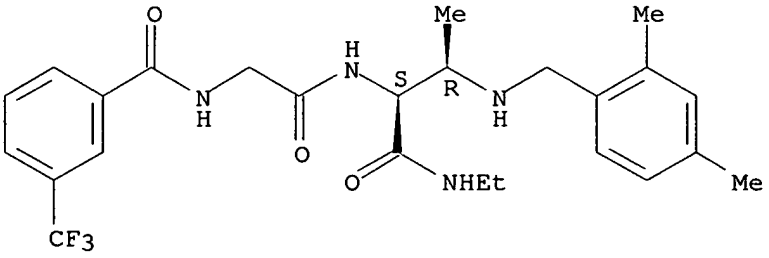
RN 439150-35-3 CAPLUS
CN Benzamide, N-[2-[[(1R)-3-[(1,1-dimethylethyl)amino]-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-3-oxopropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



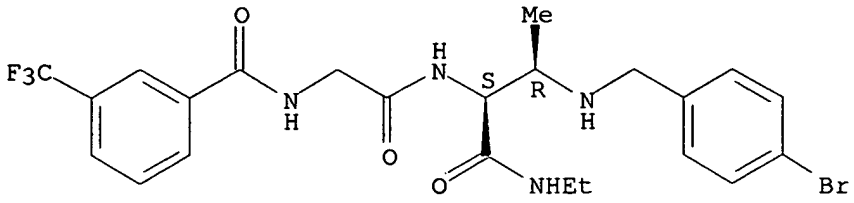
RN 439150-36-4 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-[(ethylamino)carbonyl]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



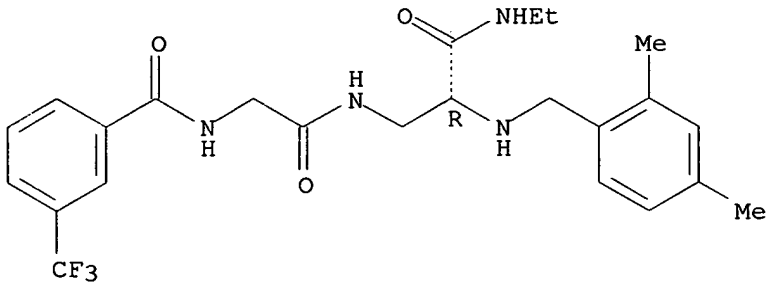
RN 439150-37-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-2-[[(4-bromophenyl)methyl]amino]-1-[(ethylamino)carbonyl]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



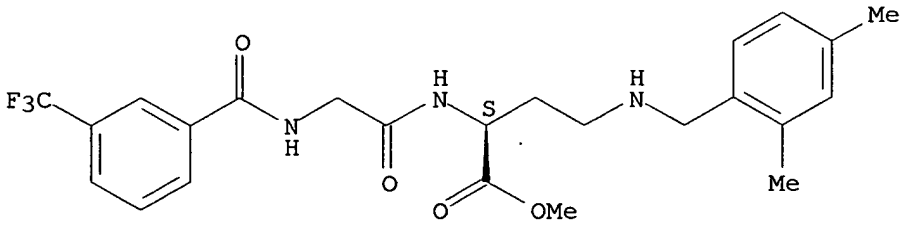
RN 439150-39-7 CAPLUS
CN Benzamide, N-[2-[[(2R)-2-[[(2,4-dimethylphenyl)methyl]amino]-3-(ethylamino)-3-oxopropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



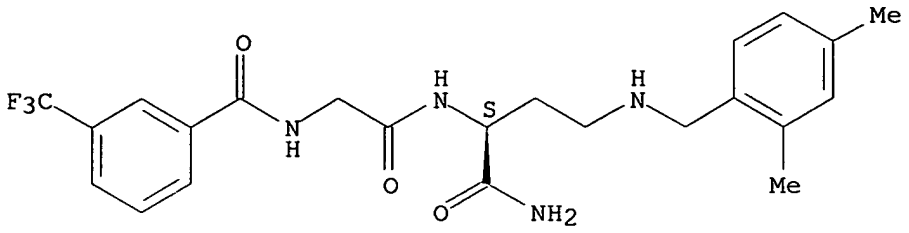
RN 439150-40-0 CAPLUS
CN Butanoic acid, 4-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]-, methyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



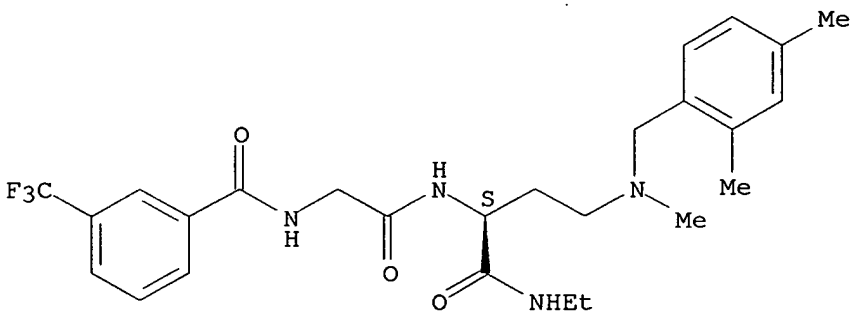
RN 439150-41-1 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-(aminocarbonyl)-3-[[(2,4-dimethylphenyl)methyl]amino]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



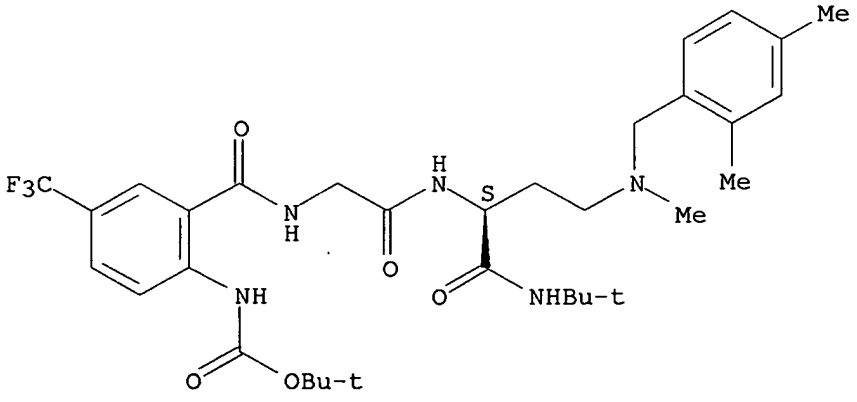
RN 439150-43-3 CAPLUS
CN Benzamide, N-[2-[[(1S)-3-[[(2,4-dimethylphenyl)methyl]methylamino]-1-[(ethylamino)carbonyl]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439150-45-5 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(2,4-dimethylphenyl)methyl]methylamino]propyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

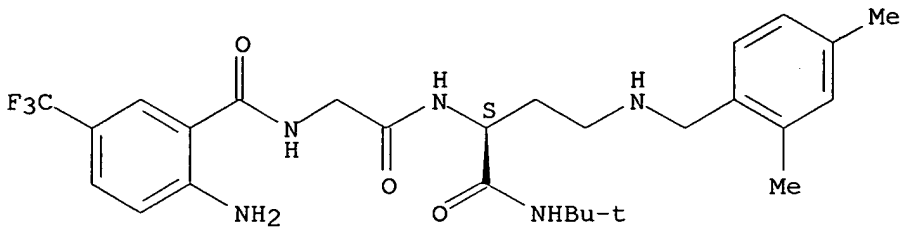
Absolute stereochemistry.



RN 439150-46-6 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(2,4-dimethylphenyl)methyl]amino]propyl]amino]-2-oxoethyl]-5-

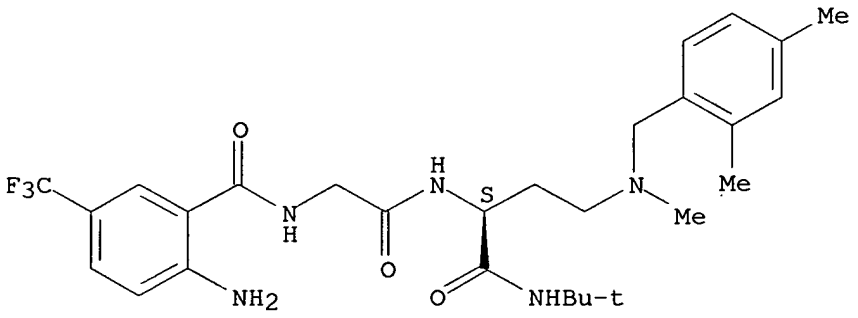
(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



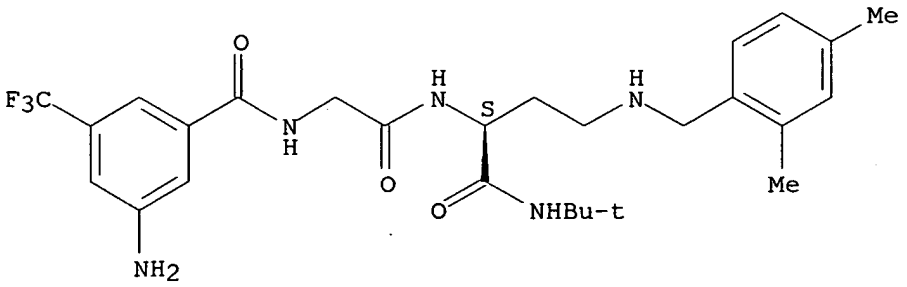
RN 439150-47-7 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(2,4-dimethylphenyl)methyl]methylamino]propyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



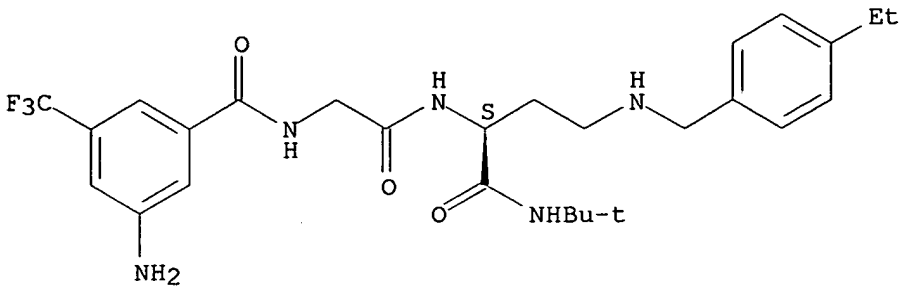
RN 439150-48-8 CAPLUS
CN Benzamide, 3-amino-N-[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(2,4-dimethylphenyl)methyl]amino]propyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



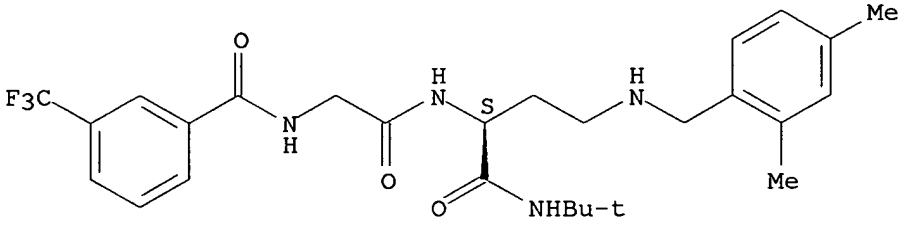
RN 439150-49-9 CAPLUS
CN Benzamide, 3-amino-N-[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(4-ethylphenyl)methyl]amino]propyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



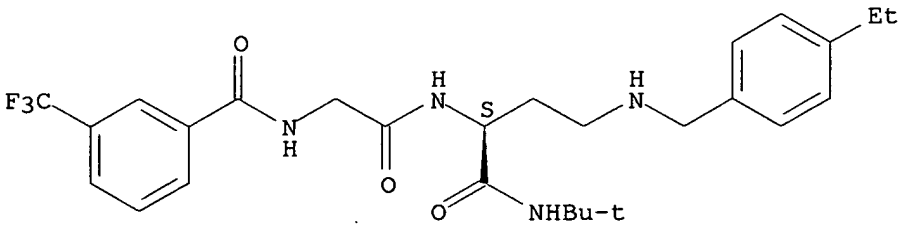
RN 439150-50-2 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(2,4-dimethylphenyl)methyl]amino]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



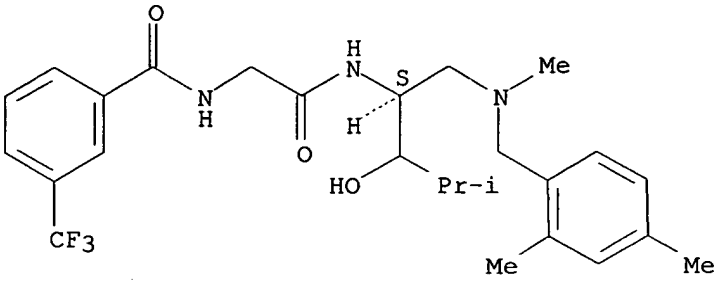
RN 439150-51-3 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[(1,1-dimethylethyl)amino]carbonyl]-3-[[(4-ethylphenyl)methyl]amino]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



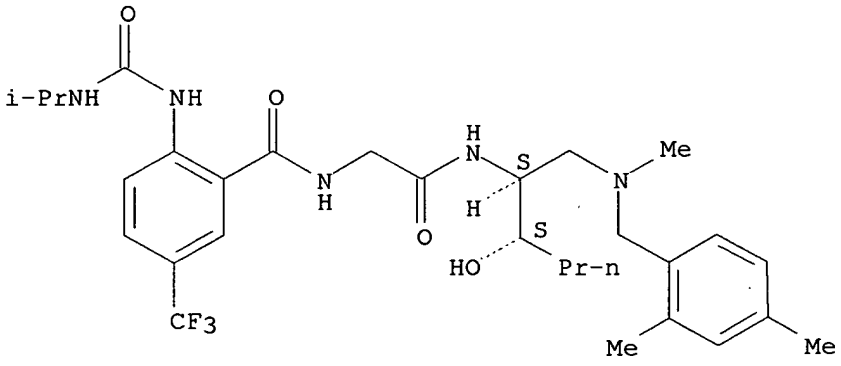
RN 439150-53-5 CAPLUS
CN D-glycero-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]methylamino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]-, (3.xi.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



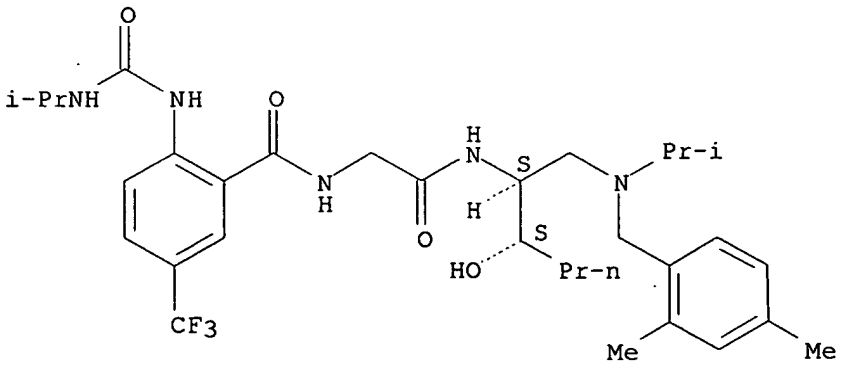
RN 439150-54-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]methylamino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



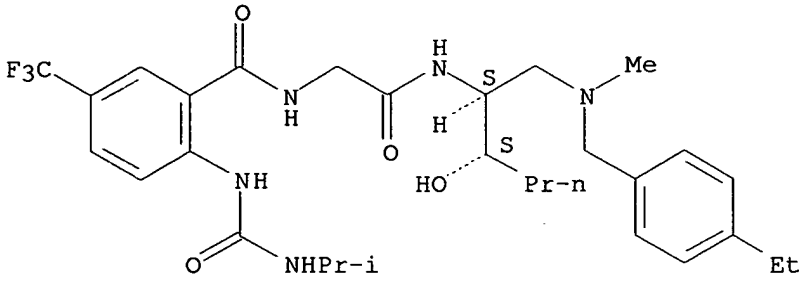
RN 439150-55-7 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl](1-methylethyl)amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



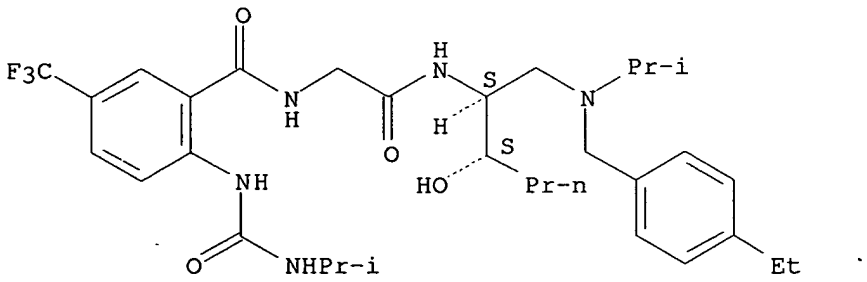
RN 439150-56-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]methylamino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



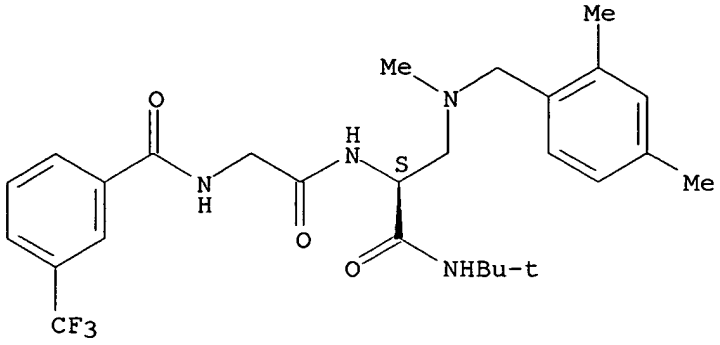
RN 439150-57-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl](1-methylethyl)amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

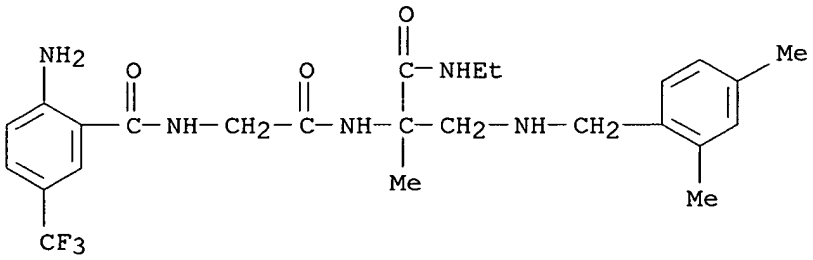


RN 439150-58-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

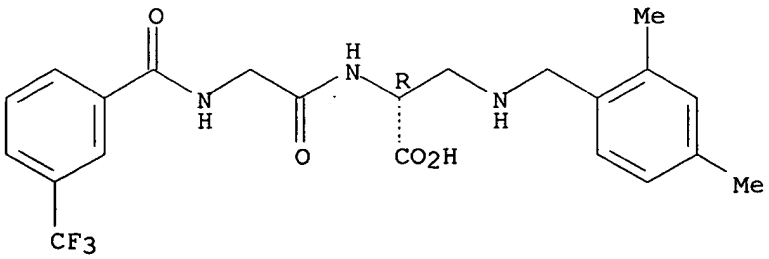


RN 439150-65-9 CAPLUS
CN Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-2-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-N-ethyl- (9CI) (CA INDEX NAME)



IT **439150-68-2P 439150-69-3P 439150-86-4P**
439150-88-6P 439150-90-0P 439150-92-2P
439151-00-5P 439151-01-6P 439151-31-2P
439151-39-0P 439151-84-5P 439152-00-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)
RN 439150-68-2 CAPLUS
CN D-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

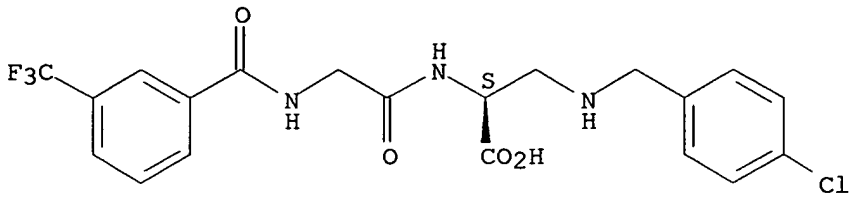
Absolute stereochemistry.



RN 439150-69-3 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-

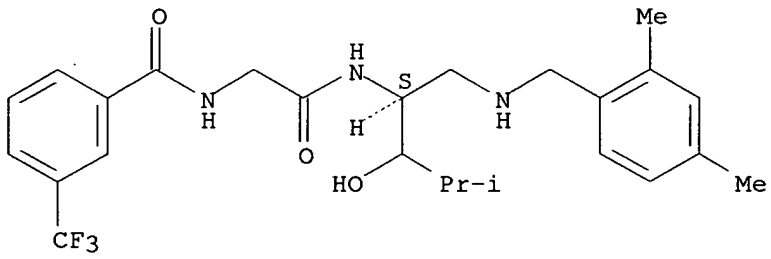
chlorophenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



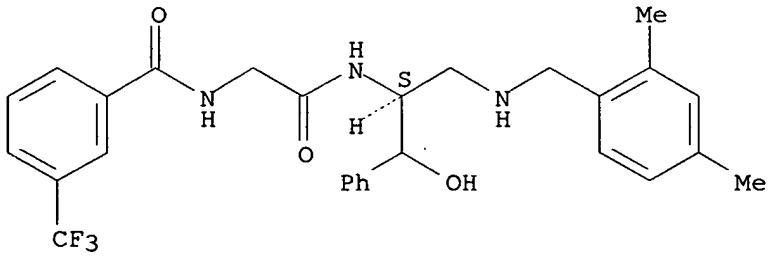
RN 439150-86-4 CAPLUS
CN D-glycero-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]-, (3.xi.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



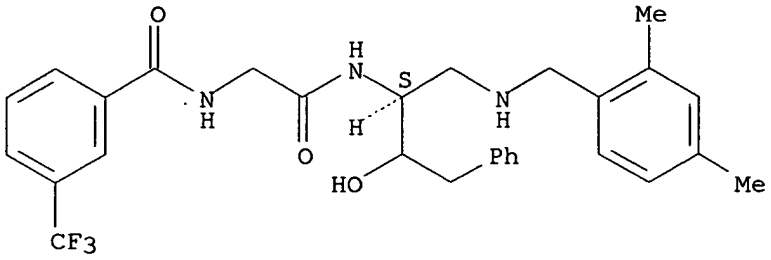
RN 439150-88-6 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



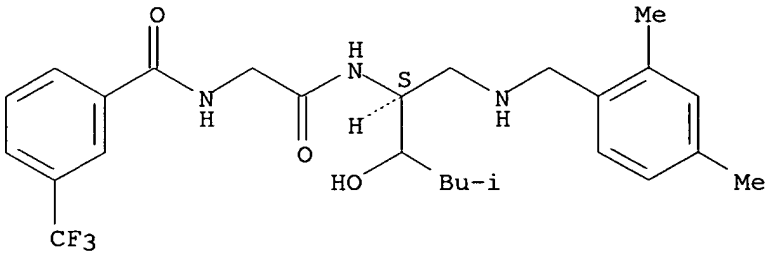
RN 439150-90-0 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-3-phenylpropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



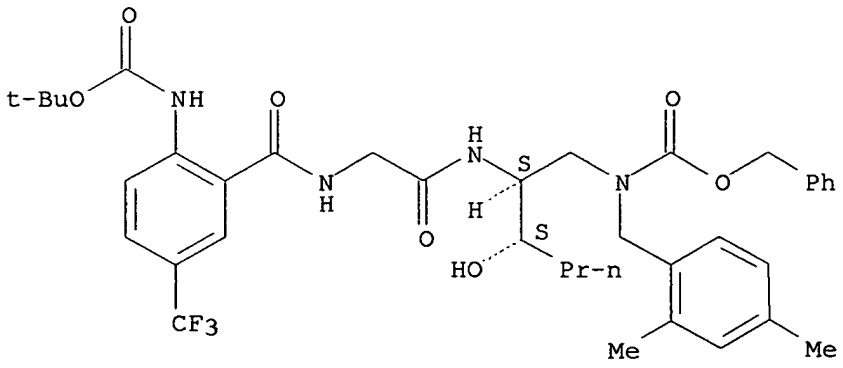
RN 439150-92-2 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



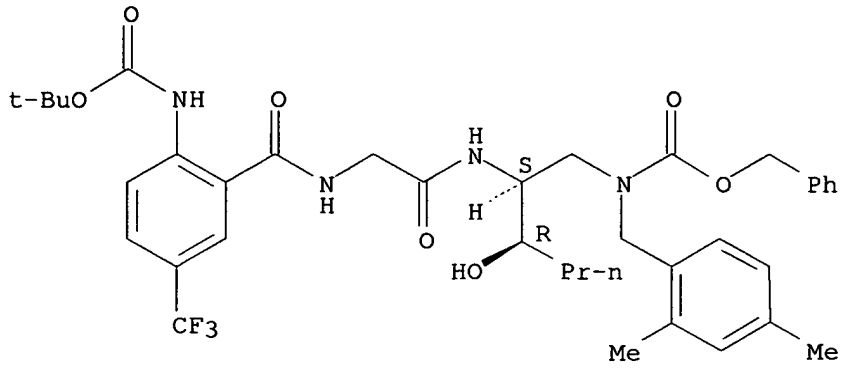
RN 439151-00-5 CAPLUS
CN Carbamic acid, [(2S,3S)-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-3-hydroxyhexyl][(2,4-dimethylphenyl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



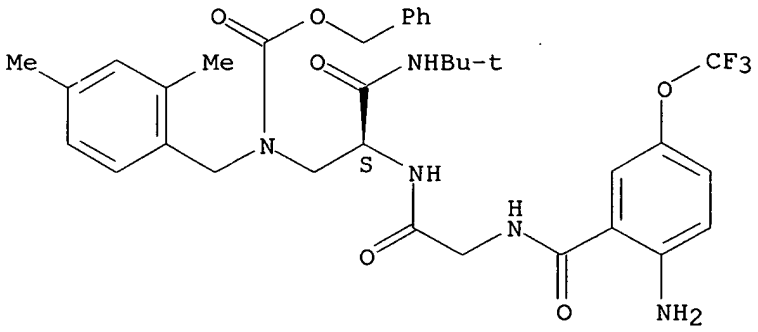
RN 439151-01-6 CAPLUS
CN Carbamic acid, [(2S,3R)-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-3-hydroxyhexyl][(2,4-dimethylphenyl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



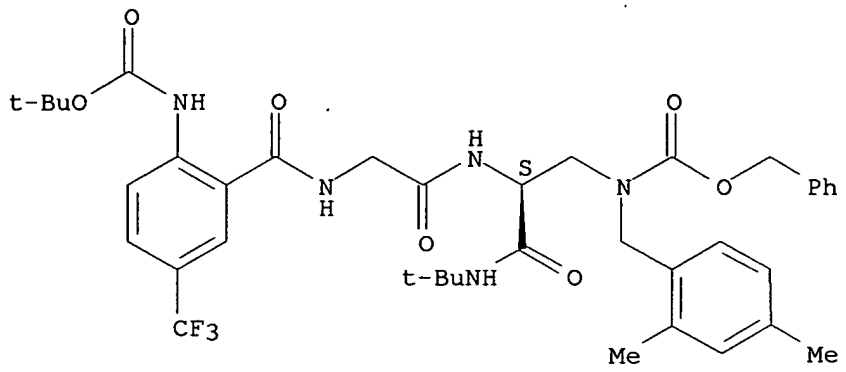
RN 439151-31-2 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethoxy)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl][(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



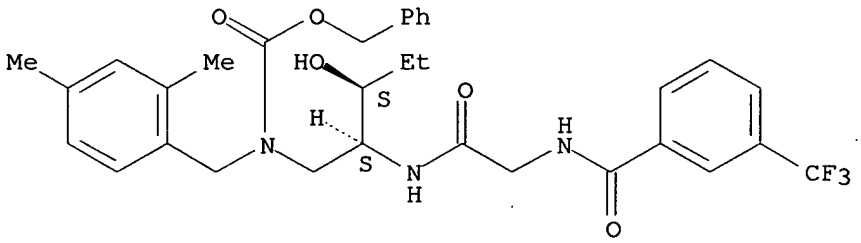
RN 439151-39-0 CAPLUS
CN L-Alaninamide, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl][(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



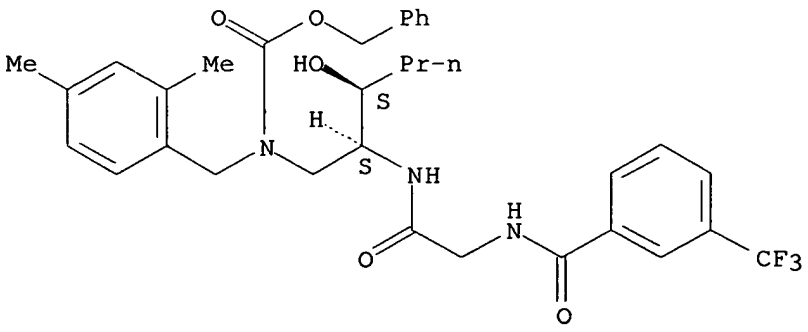
RN 439151-84-5 CAPLUS
CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl][(phenylmethoxy)carbonyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439152-00-8 CAPLUS
CN Carbamic acid, [(2,4-dimethylphenyl)methyl][(2S,3S)-3-hydroxy-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]hexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

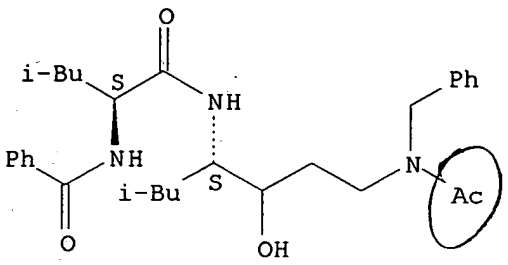


L26 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:708752 CAPLUS
DN 131:322921
TI Preparation of hydroxypropylamide peptidomimetics as inhibitors of aspartyl proteases
IN Dolle, Roland Ellwood, III; Cavallaro, Cullen Lee; Herpin, Timothee Felix
PA Pharmacopeia, Inc., USA
SO PCT Int. Appl., 48 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9955687	A2	19991104	WO 1999-US9070	19990427
	WO 9955687	A3	20000224		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 5986102	A	19991116	US 1998-69380	19980429
	AU 9938684	A1	19991116	AU 1999-38684	19990427
	US 6191277	B1	20010220	US 1999-408237	19990929
PRAI	US 1998-69380	A	19980429		
	WO 1999-US9070	W	19990427		

OS MARPAT 131:322921
AB Compds. Z-NR2CHR1CH(OH)CH2CH2-Y [R1 = alkyl, -(CH2)n-cycloalkyl (n = 1-3), aralkyl; R2 = H or [S]-CO-L-, where [S] is a solid support and -L- is a linker; Y = O2CNHR3 or NR4R5, where R3 is alkyl, aralkyl, aryl, or aryloxyalkyl and R4 and R5 are independently H, alkoxyalkyl, R3, COR3, SO2R3, 2-indanyl(CH2)m (m = 0-3) or R4R5N is morpholino or N-substituted 1-piperazinyl; Z = COR7, COCHR8O2CNHR3, COCHR8NHCOR3, where R7 is alkyl, aralkyl, aryl, -(CH2)m-cycloalkyl, heteroaryl, 1-(carboxy ester)-2-pyrrolidinyl, 2-indanyl-(CH2)n and R8 = H, alkyl, aralkyl, -(CH2)m-cycloalkyl] were prepd. as inhibitors having activity against the aspartyl proteases plasmepsin and cathepsin D. Thus, compd. I was prepd. by the solid-phase method and shown to inhibit plasmepsin or cathepsin D at a concn. (IC50) of less than 350 micromolar.
IT **248596-87-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of hydroxypropylamide peptidomimetics as inhibitors of aspartyl proteases)
RN 248596-87-4 CAPLUS
CN Benzamide, N-[(1S)-1-[[[(1S)-4-[acetyl(phenylmethyl)amino]-2-hydroxy-1-(2-methylpropyl)butyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

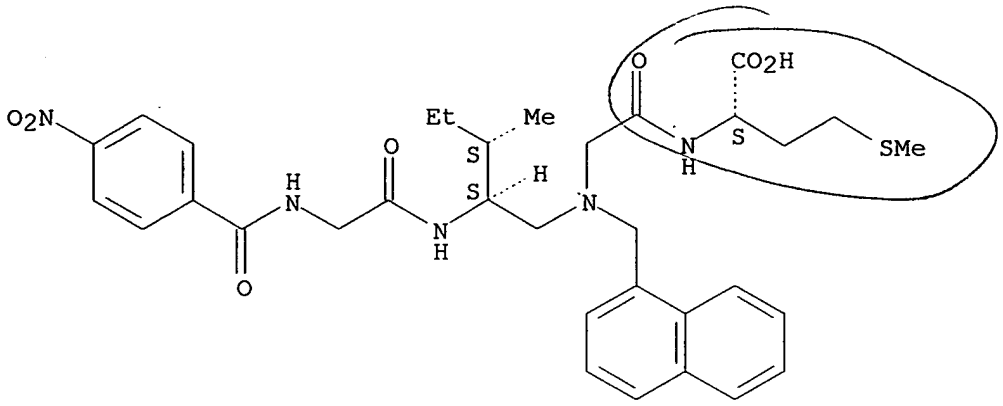

O
i-Bu
S
NH
Ph
Ph
NH
N
i-Bu
S
Ac
O
OH

L26 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:397225 CAPLUS
DN 125:76352
TI Tetrapeptide-based inhibitors of farnesyl protein transferase
IN Breslin, Michael J.; Desolms, S. Jane; Graham, Samuel L.; Hutchinson, John H.; Stokker, Gerald E.
PA Merck and Co., Inc., USA
SO PCT Int. Appl., 168 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9609836	A1	19960404	WO 1995-US12319	19950925
	W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UG, US, UZ				
	RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 5585359	A	19961217	US 1994-315171	19940929
	AU 9536425	A1	19960419	AU 1995-36425	19950925
	AU 708986	B2	19990819		
	EP 783318	A1	19970716	EP 1995-933956	19950925
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	JP 10506897	T2	19980707	JP 1995-511979	19950925
PRAI	US 1994-315171		19940929		
	WO 1995-US12319		19950925		

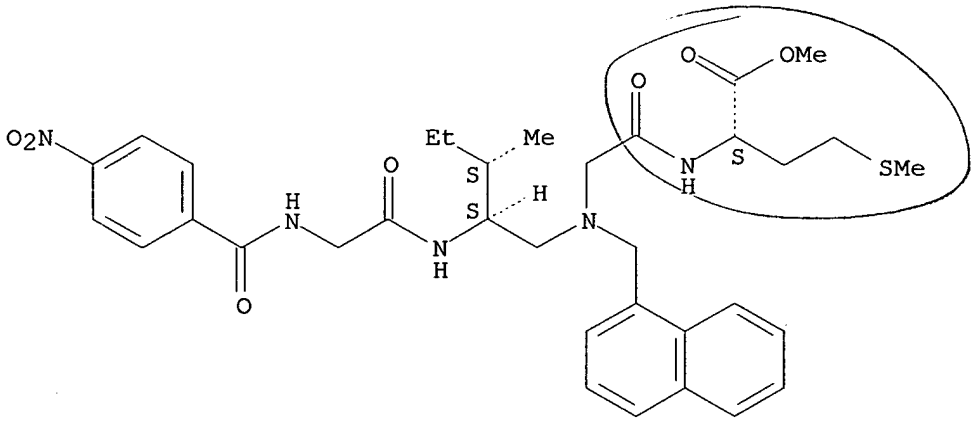
OS MARPAT 125:76352
AB The title inhibitors comprise analogs of the CAAX motif of protein Ras that is modified by farnesylation in vivo. These CAAX analogs inhibit the farnesylation of Ras and are potentially useful as antitumor agents. Furthermore, these CAAX analogs differ from those previously described as inhibitors of Ras farnesyl transferase in that they do not have a thiol moiety. The lack of the thiol offers unique advantages in terms of improved pharmacokinetic behavior in animals, prevention of thiol-dependent chem. reactions (e.g. rapid autoxidn. and disulfide formation with endogenous thiols), and reduced systemic toxicity. Thus, N-[2(S)-[(4-nitrobenzylthio)acetamido]-3(S)-methylpentyl]-N-(1-naphthylmethyl)glycylmethionine (I) and related compds. inhibited bovine farnesyl protein transferase in vitro with IC50 <10 .mu.M. I was prepd. by successive condensation of glycine Me ester-HCl with N-tert-butoxycarbonylisoleucinal, 1-naphthaldehyde, methionine Me ester-HCl, and (4-nitrobenzylthio)acetic acid with deprotection at appropriate stages.
IT **178270-23-0P 178270-24-1P 178270-25-2P**
178270-26-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(tetrapeptide-based inhibitors of farnesyl protein transferase)
RN 178270-23-0 CAPLUS
CN L-Methionine, N-[N-[3-methyl-2-[[[(4-nitrobenzoyl)amino]acetyl]amino]pentyl]-N-(1-naphthalenylmethyl)glycyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



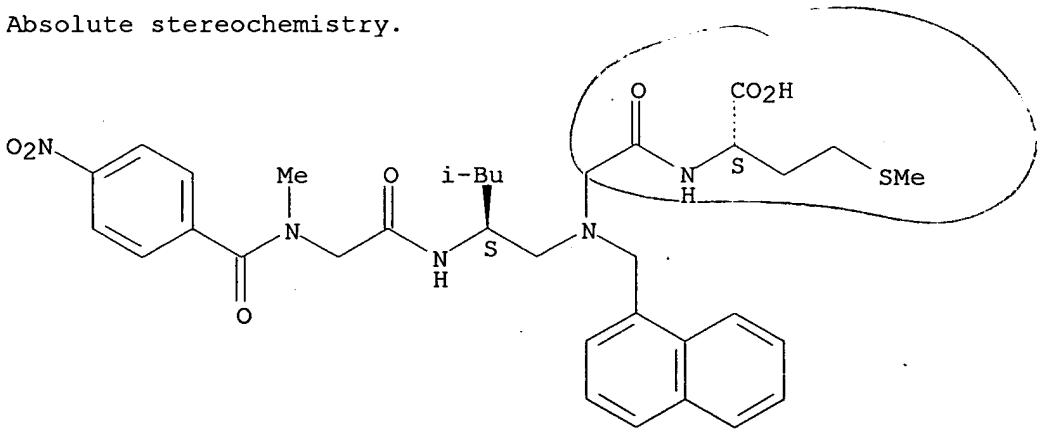
RN 178270-24-1 CAPLUS
CN L-Methionine, N-[N-[3-methyl-2-[[[(4-nitrobenzoyl)amino]acetyl]amino]pentyl]-N-(1-naphthalenylmethyl)glycyl]-, methyl ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 178270-25-2 CAPLUS
CN L-Methionine, N-[N-[4-methyl-2-[[[methyl(4-nitrobenzoyl)amino]acetyl]amino]pentyl]-N-(1-naphthalenylmethyl)glycyl]-, (S)- (9CI) (CA INDEX NAME)

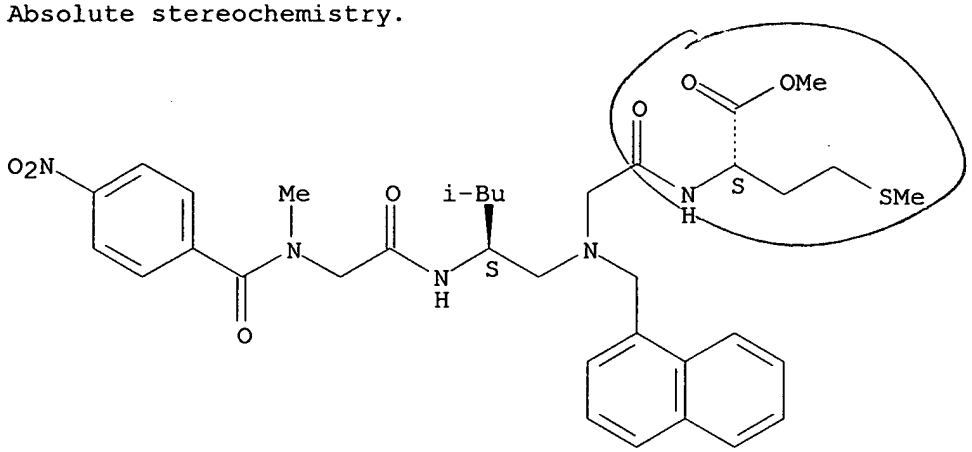
Absolute stereochemistry.



RN 178270-26-3 CAPLUS
CN L-Methionine, N-[N-[4-methyl-2-[[[methyl(4-nitrobenzoyl)amino]acetyl]amino

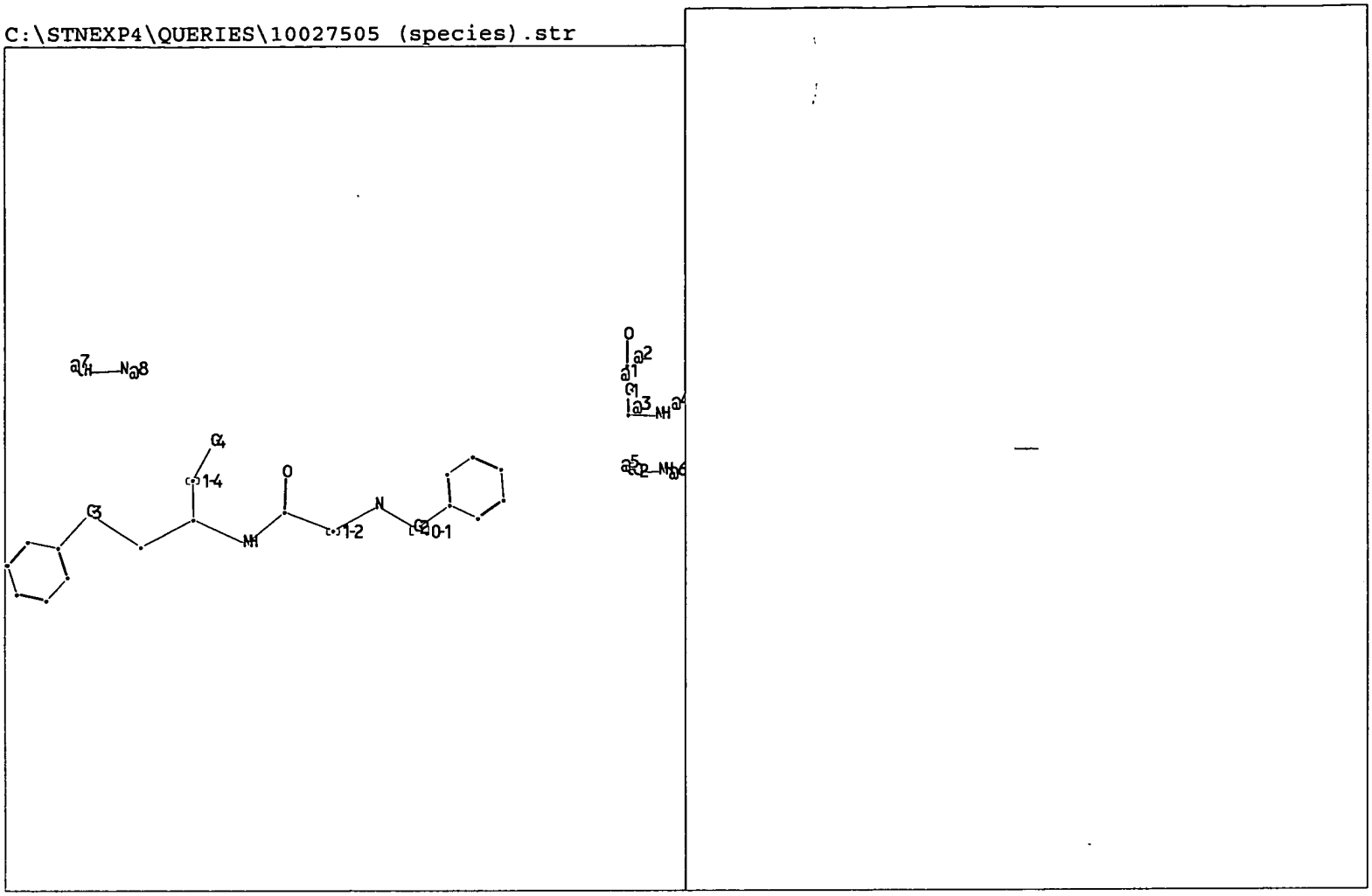
]pentyl]-N-(1-naphthalenylmethyl)glycyl]-, methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



```
=> d his

     (FILE 'HOME' ENTERED AT 10:19:32 ON 29 DEC 2003)

     FILE 'REGISTRY' ENTERED AT 10:19:41 ON 29 DEC 2003
L1             STRUCTURE UPLOADED
L2           0 S L1 SSS SAM
L3             STRUCTURE UPLOADED
L4           0 S L3 SSS SAM
L5             SCREEN 1839
L6             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L7             STRUCTURE UPLOADED
L8             QUE L7 AND L5 NOT L6
L9           1 S L8 SSS SAM
L10            SCREEN 1839 AND 1994
L11            SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L12            STRUCTURE UPLOADED
L13            QUE L12 AND L10 NOT L11
L14          3 S L13 SSS SAM
L15            SCREEN 1839
L16            SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L17            STRUCTURE UPLOADED
L18            QUE L17 AND L15 NOT L16
L19          0 S L18 SSS SAM
L20            SCREEN 1839
L21            SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L22            STRUCTURE UPLOADED
L23            QUE L22 AND L20 NOT L21
L24          1 S L23 SSS SAM
L25        243 S L23 SSS FUL

     FILE 'CAPLUS' ENTERED AT 10:33:56 ON 29 DEC 2003
L26          6 S L25

     FILE 'CAOLD' ENTERED AT 10:34:42 ON 29 DEC 2003

=> s l25
L27          0 L25

=> log y
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                  ENTRY    SESSION
FULL ESTIMATED COST                                0.40     185.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)      SINCE FILE      TOTAL
                                                  ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -3.91

STN INTERNATIONAL LOGOFF AT 10:34:53 ON 29 DEC 2003
```

C:\STNEXP4\QUERIES\10027505 (species).str



chain nodes :
2 3 4 5 6 7 8 10 11 21 22 25 26 27 28 29 30 31 36 38
ring nodes :
1 35 41 42 43 44 45 46 47 48 49 50
chain bonds :
1-2 2-3 3-21 4-5 6-7 6-10 8-11 21-22 22-25 22-26 26-27 27-36 27-28 28-29
29-35 30-31 36-38
ring bonds :
1-41 1-45 35-46 35-50 41-42 42-43 43-44 44-45 46-47 47-48 48-49 49-50
exact/norm bonds :
1-2 2-3 3-21 4-5 6-7 6-10 8-11 22-25 22-26 26-27 28-29 29-35 30-31 36-38
exact bonds :
21-22 27-36 27-28
normalized bonds :
1-41 1-45 35-46 35-50 41-42 42-43 43-44 44-45 46-47 47-48 48-49 49-50
isolated ring systems :
containing 1 : 35 :

G1:O,S

G2:SO2,[*1-*2],[*3-*4],[*5-*6]

G3:O,S,N,[*7-*8]

G4:C,O,S,N,Cy

Match level :
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 10:CLASS 11:CLASS
21:CLASS 22:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS
35:Atom 36:CLASS 38:CLASS 41:CLASS 42:CLASS 43:Atom 44:Atom 45:Atom 46:Atom
47:Atom 48:Atom 49:Atom 50:Atom

```
=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L1    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L2    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505.str

L3      STRUCTURE UPLOADED

=> que L3 AND L1 NOT L2

L4   QUE L3 AND L1 NOT L2

=> d l4
L4 HAS NO ANSWERS
L1              SCR 1839
L2              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L3              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L4              QUE  L3 AND L1 NOT L2


=> s l4 sss sam
SAMPLE SEARCH INITIATED 18:37:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  51181 TO ITERATE

  2.0% PROCESSED    1000 ITERATIONS                                7 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS    6030

L5            7 SEA SSS SAM L3 AND L1 NOT L2

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L6    SCREEN CREATED
```

```
=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L7    SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505.str

L8      STRUCTURE UPLOADED

=> que L8 AND L6 NOT L7

L9   QUE L8 AND L6 NOT L7

=> d 19
L9 HAS NO ANSWERS
L6              SCR 1839
L7              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L8              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L9              QUE  L8 AND L6 NOT L7


=> s 19 sss sam
SAMPLE SEARCH INITIATED 18:39:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  51181 TO ITERATE

  2.0% PROCESSED    1000 ITERATIONS                              4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS    3236

L10           4 SEA SSS SAM L8 AND L6 NOT L7

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L11   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L12   SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505.str

L13     STRUCTURE UPLOADED
```

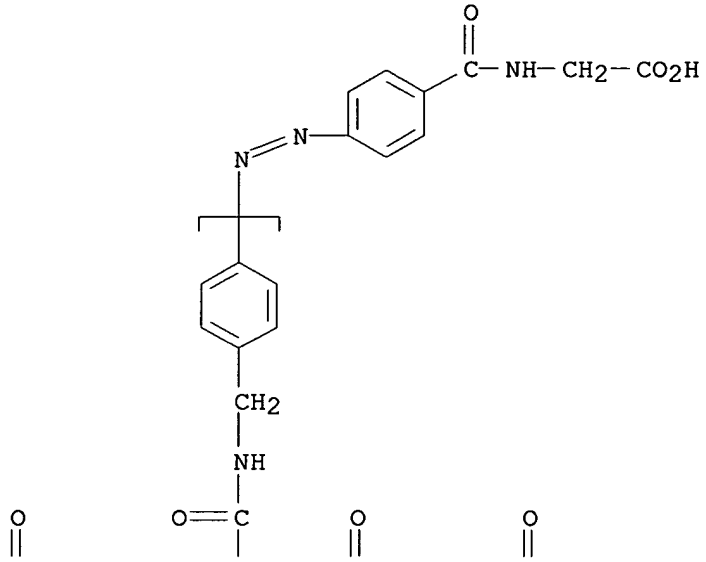
```
=> que L13 AND L11 NOT L12

L14  QUE L13 AND L11 NOT L12

=> d l14
L14 HAS NO ANSWERS
L11             SCR 1839
L12             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L13             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L14             QUE  L13 AND L11 NOT L12


=> s l14 sss sam
SAMPLE SEARCH INITIATED 18:43:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  51181 TO ITERATE

  2.0% PROCESSED    1000 ITERATIONS                              1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS     594

L15           1 SEA SSS SAM L13 AND L11 NOT L12

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L16   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L17   SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505.str

L18     STRUCTURE UPLOADED

=> que L18 AND L16 NOT L17

L19  QUE L18 AND L16 NOT L17

=> d l19
L19 HAS NO ANSWERS
L16             SCR 1839
L17             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L18             STR
```

```
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L19             QUE  L18 AND L16 NOT L17


=> s l19 sss sam
SAMPLE SEARCH INITIATED 18:44:59 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  77851 TO ITERATE

  1.3% PROCESSED    1000 ITERATIONS                                1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS    1028

L20           1 SEA SSS SAM L18 AND L16 NOT L17

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L21   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L22   SCREEN CREATED

=>
Uploading C:\STNEXP4\QUERIES\10027505 (species).str

L23     STRUCTURE UPLOADED

=> que L23 AND L21 NOT L22

L24  QUE L23 AND L21 NOT L22

=> d l24
L24 HAS NO ANSWERS
L21             SCR 1839
L22             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L23             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L24             QUE  L23 AND L21 NOT L22


=> s l24 sss sam
SAMPLE SEARCH INITIATED 18:48:02 FILE 'REGISTRY'
```

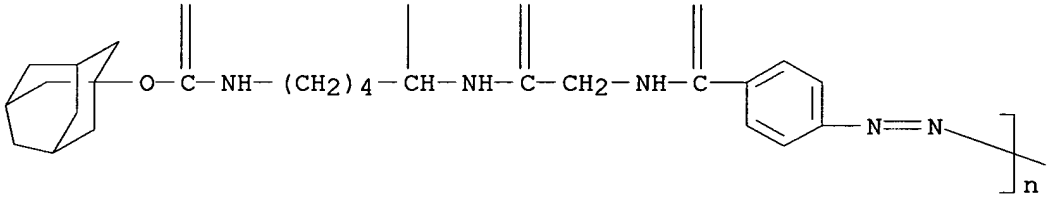
```
SAMPLE SCREEN SEARCH COMPLETED -   9265 TO ITERATE

 10.8% PROCESSED    1000 ITERATIONS                                4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       179536 TO   191064
PROJECTED ANSWERS:             376 TO     1106

L25           4 SEA SSS SAM L23 AND L21 NOT L22

=> s l24 sss ful
FULL SEARCH INITIATED 18:49:03 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 186868 TO ITERATE

100.0% PROCESSED  186868 ITERATIONS                            356 ANSWERS
SEARCH TIME: 00.00.13

L26         356 SEA SSS FUL L23 AND L21 NOT L22

=> s l26
L27          84 L26

=> d l27 1-40 bib,ab,hitstr
```

L27 ANSWER 1 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2003:139800 CAPLUS
DN 138:321666
TI Single Molecule Force Spectroscopy of Azobenzene Polymers: Switching Elasticity of Single Photochromic Macromolecules
AU Holland, Nolan B.; Hugel, Thorsten; Neuert, Gregor; Cattani-Scholz, Anna; Renner, Christian; Oesterhelt, Dieter; Moroder, Luis; Seitz, Markus; Gaub, Hermann E.
CS Lehrstuhl fuer Angewandte Physik Center for Nanoscience, Ludwig-Maximilians-Universitaet, Munich, 80799, Germany
SO Macromolecules (2003), 36(6), 2015-2023
CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal
LA English
AB The reversible, optical switching of individual mols. of a polypeptide with azobenzene moieties, was obsd. using mol. force spectroscopy. The polypeptide was prepd. by polycondensation of tripeptide monomers contg. (4-aminomethyl)phenylazobenzoic acid (AMPB) to obtain H-Cys(Trt)-[Lys(Adoc)-AMPB-Gly]n-OH. The contour length of the polymer could be selectively lengthened or shortened by switching between the trans- and cis-azo configurations with 420 and 365 nm wavelength light, resp. This cis- to trans-azo configurational transition induced by UV light resulted in a measurable change in polymer contour length. The contour length change was obsd. at low force and under external loads of up to 400 pN using a modified force spectrometer, in which the sample could be irradiated in total internal reflectance. The ability to shorten the polymer against an external load demonstrates photomech. energy conversion in an individual mol., of interest in development of mol. machines.
IT **512197-45-4P**
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation) (switching elasticity of polypeptide-azobenzene single photochromic mols. studied by optical excitation and AFM using object slide as waveguide)
RN 512197-45-4 CAPLUS
CN Poly[(1E)-azo-1,4-phenylenecarbonylimino(2-oxo-1,2-ethanediyl)imino[(1S)-2-oxo-1-[4-[[(tricyclo[3.3.1.13,7]dec-1-yloxy)carbonyl]amino]butyl]-1,2-ethanediyl]iminomethylene-1,4-phenylene], .alpha.-[4-[[[S-(triphenylmethyl)-L-cysteinyl-N6-[(tricyclo[3.3.1.13,7]dec-1-yloxy)carbonyl]-L-lysyl]amino]methyl]phenyl]-.omega.-[(1E)-[4-[[(carboxymethyl)amino]carbonyl]phenyl]azo]- (9CI) (CA INDEX NAME)

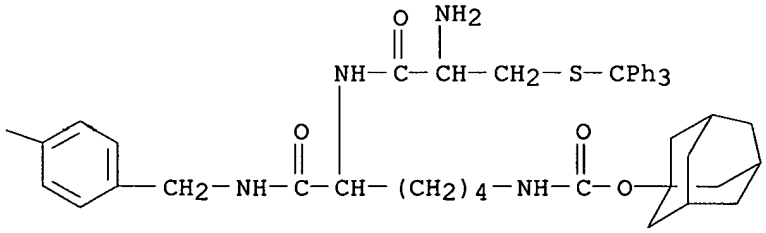
PAGE 1-A



PAGE 2-A



PAGE 2-B



RE.CNT 72 THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

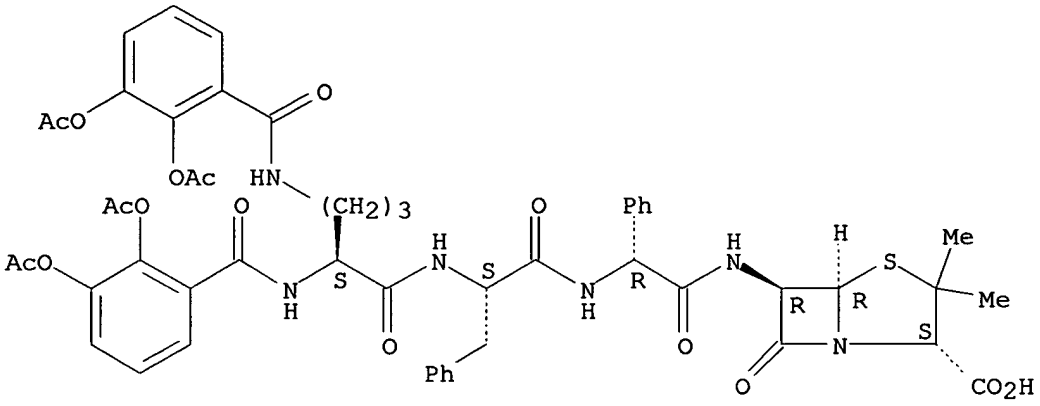
L27 ANSWER 2 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2002:671743 CAPLUS
DN 137:201608
TI Synthesis of antibacterial siderophore-amino acid/peptide-antibiotic conjugates for therapeutic use
IN Wittmann, Steffen; Heinisch, Lothar; Mollmann, Ute
PA Grunenthal GmbH, Germany
SO Ger. Offen., 10 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10111163	A1	20020905	DE 2001-10111163	20010301
	WO 2002070017	A1	20020912	WO 2002-EP2074	20020227

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

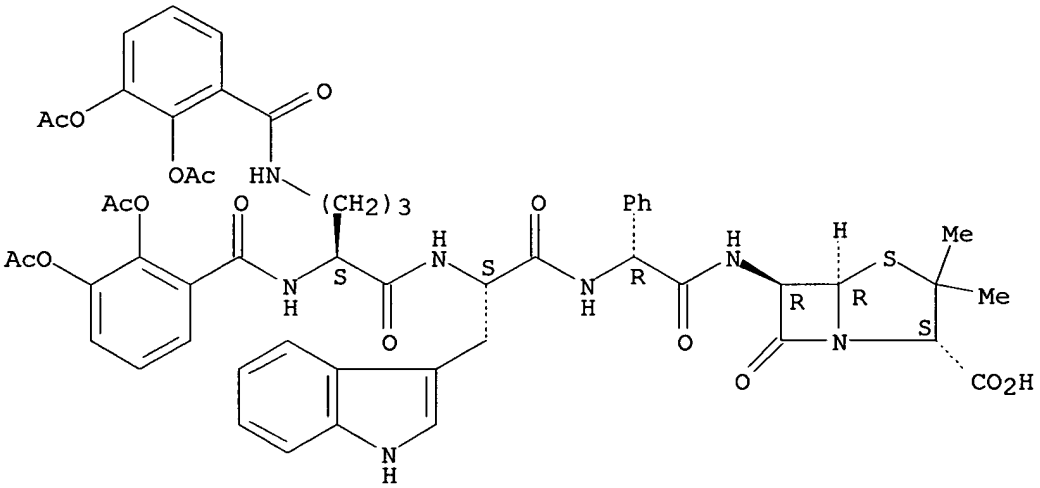
PRAI DE 2001-10111163 A 20010301
OS MARPAT 137:201608
AB The invention concerns siderophore-amino acid/peptide-antibiotic conjugates (e.g., I) capable of utilizing the bacterial iron transport mechanism for use as antibacterial agents. Thus, I was prepd. by condensation of N-[N2,N5-bis(2,3-diacetoxybenzoyl)-L-ornithinyl]-L-O-benzyl-serine and ampicillin, with further reaction to prep. the sodium salt. In antibacterial tests against a panel of organisms, title compds. had activities comparable or better than azlocillin, ampicillin, or meropenem.
IT **439152-40-6P 439152-41-7P 439152-43-9P**
439152-44-0P 439152-48-4P 439152-49-5P
439152-50-8P 439152-51-9P 454472-72-1P
454472-73-2P 454472-74-3P 454472-75-4P
454472-76-5P 454472-77-6P 454472-78-7P
454472-79-8P 454472-80-1P 454472-81-2P
454472-82-3P 454472-87-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of for use as antibacterial agents)
RN 439152-40-6 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-phenylalanyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



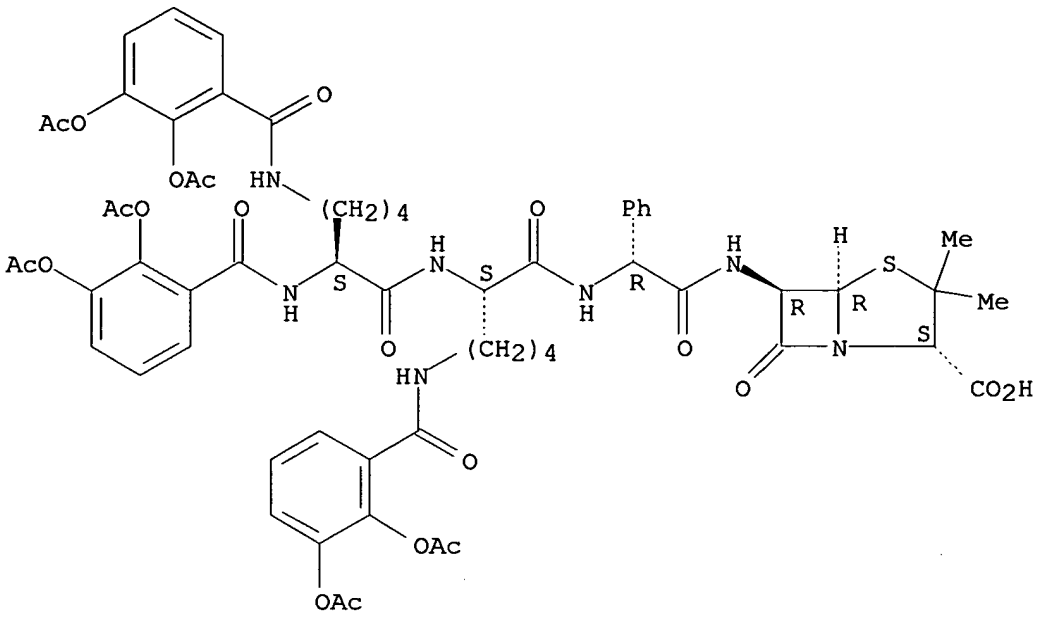
RN 439152-41-7 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-tryptophyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



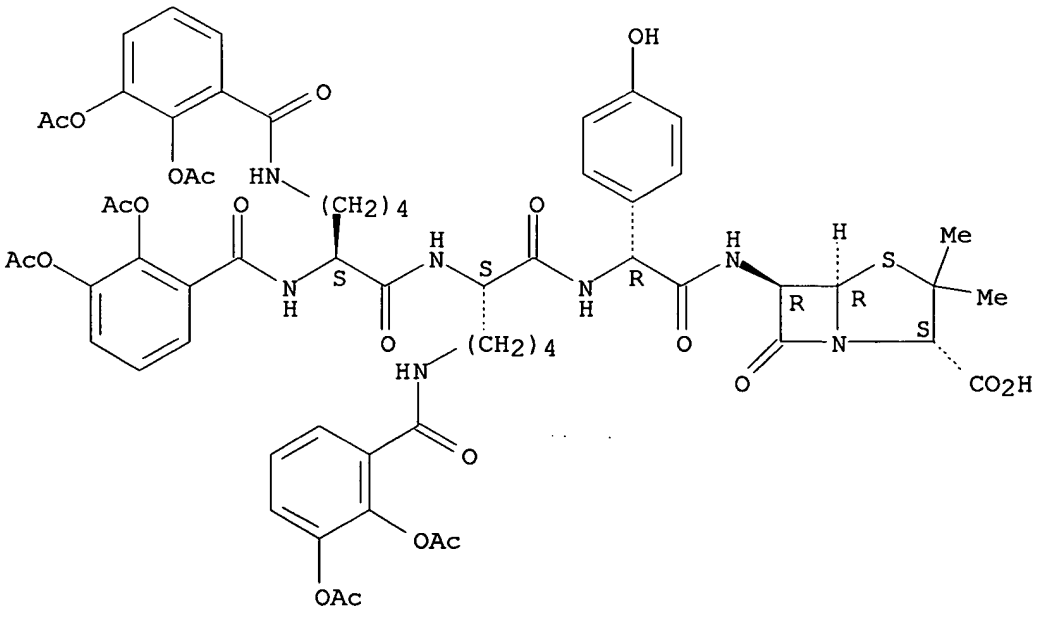
RN 439152-43-9 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N6-[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439152-44-0 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N6-[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-(4-hydroxyphenyl)-, (2R)- (9CI) (CA INDEX NAME)

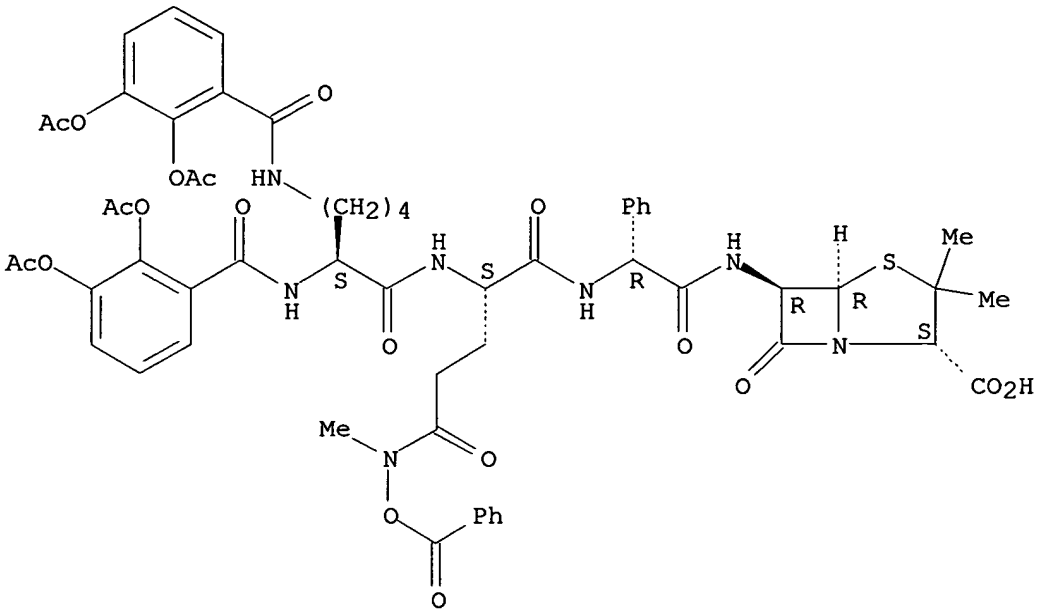
Absolute stereochemistry.



RN 439152-48-4 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-(benzoyloxy)-N-methyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-

azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

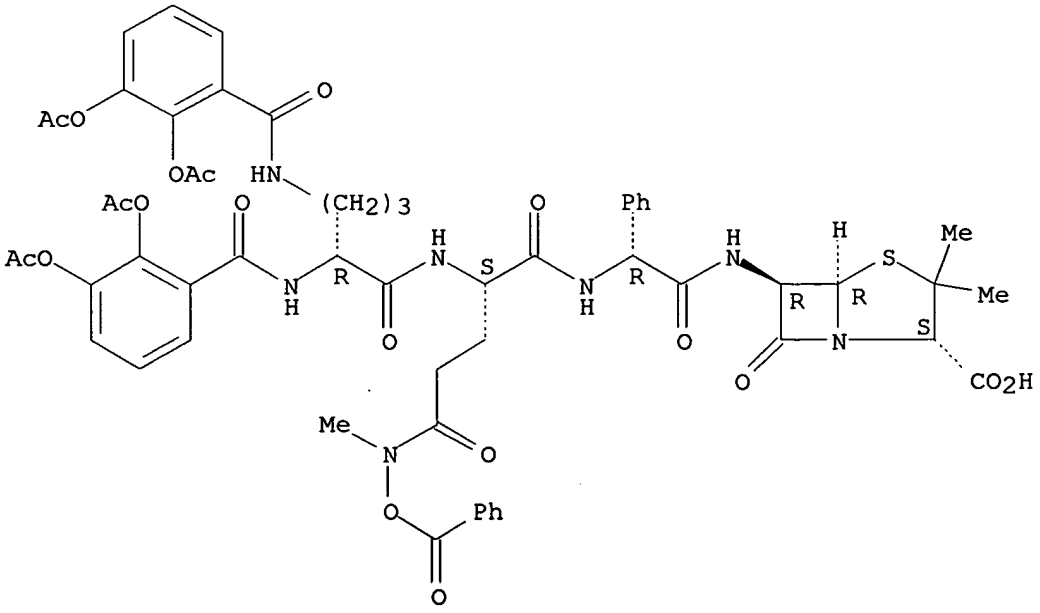
Absolute stereochemistry.



RN 439152-49-5 CAPLUS

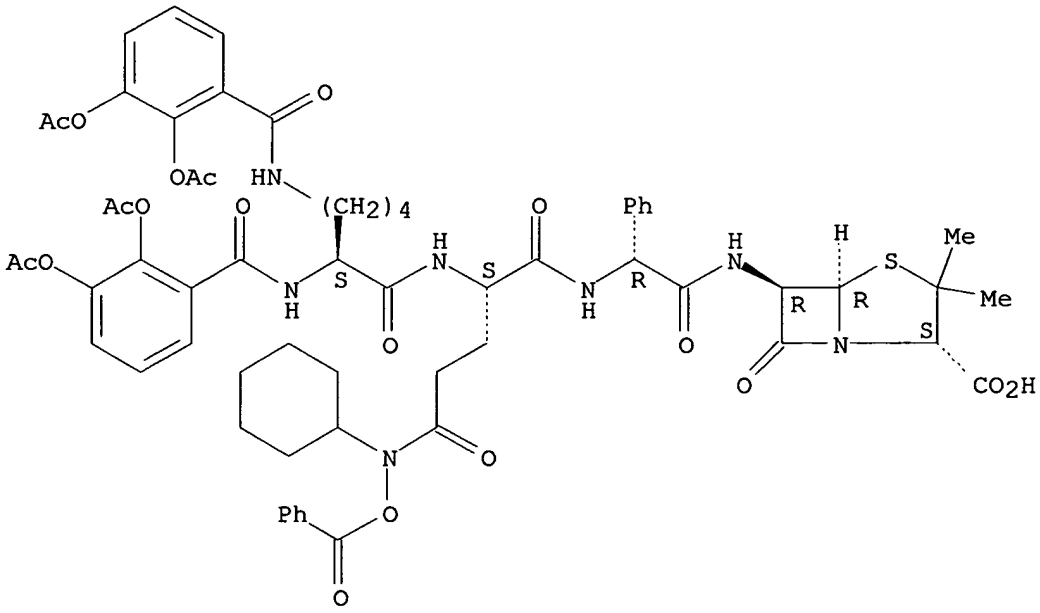
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-D-ornithyl-N-(benzoyloxy)-N-methyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



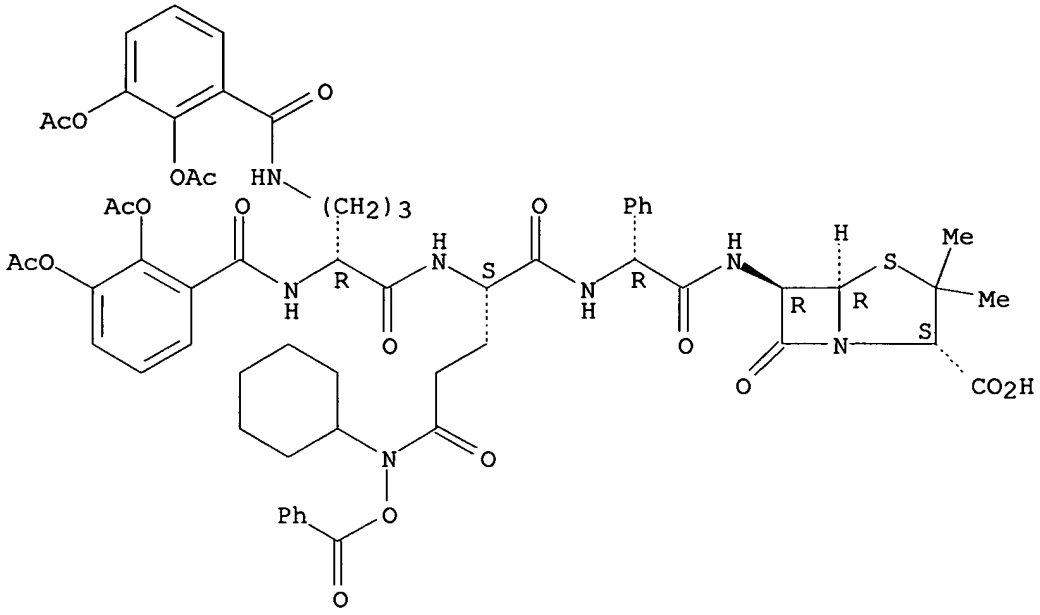
RN 439152-50-8 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-(benzoyloxy)-N-cyclohexyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



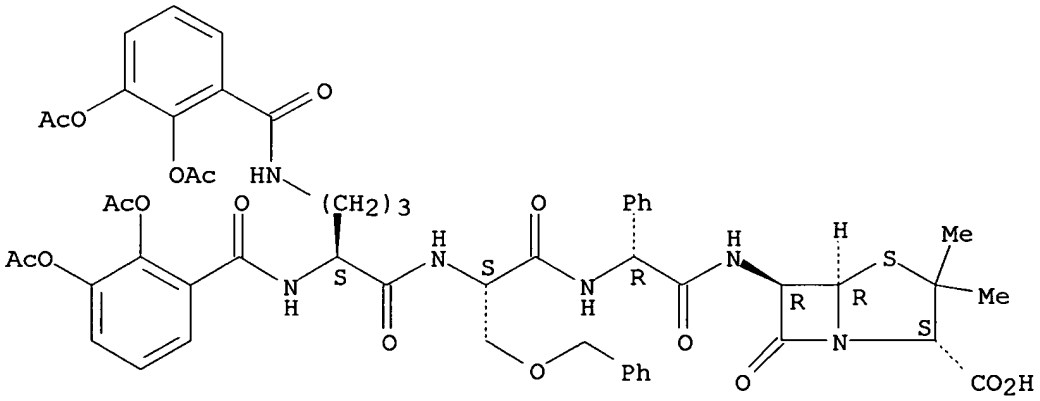
RN 439152-51-9 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-D-ornithyl-N-(benzoyloxy)-N-cyclohexyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



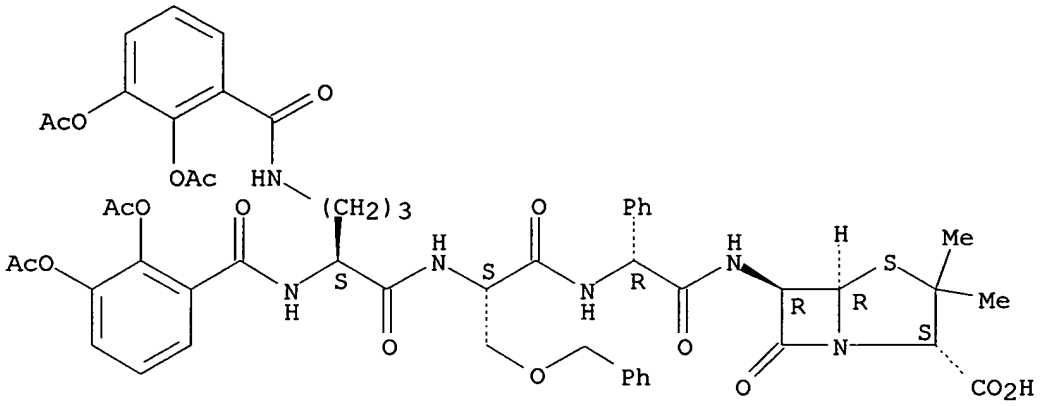
RN 454472-72-1 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-O-(phenylmethyl)-L-seryl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 454472-73-2 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-O-(phenylmethyl)-L-seryl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

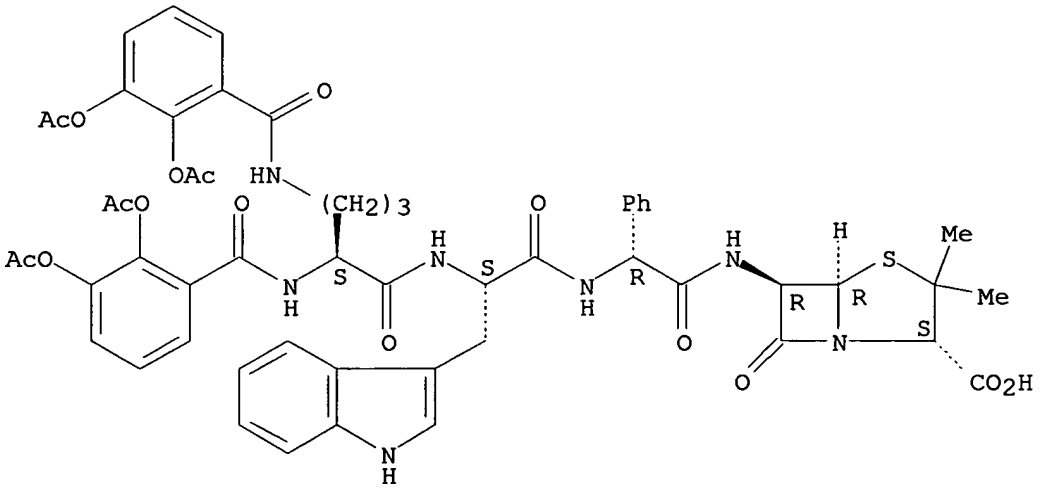
Absolute stereochemistry.



● Na

RN 454472-74-3 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-tryptophyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

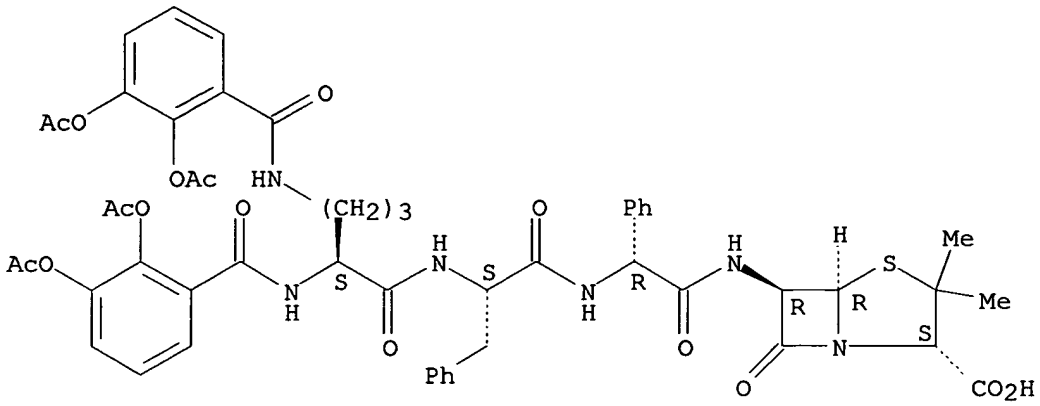
Absolute stereochemistry.



● Na

RN 454472-75-4 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-phenylalanyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

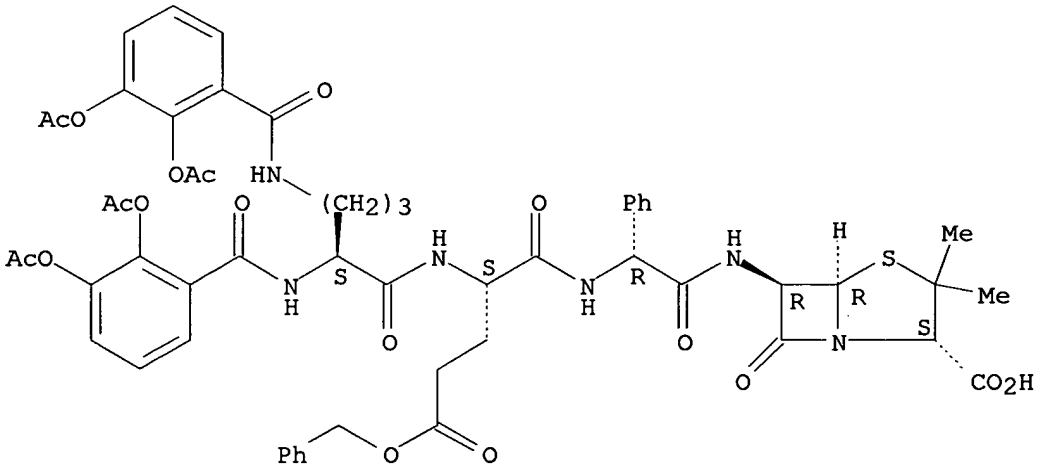
Absolute stereochemistry.



● Na

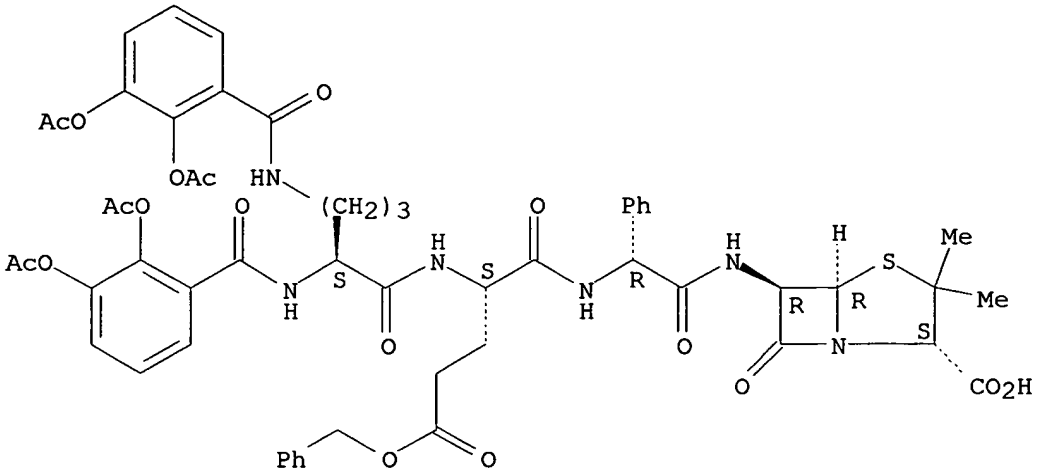
RN 454472-76-5 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-.alpha.-glutamyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, 2-(phenylmethyl) ester, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 454472-77-6 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-.alpha.-glutamyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, 2-(phenylmethyl) ester, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

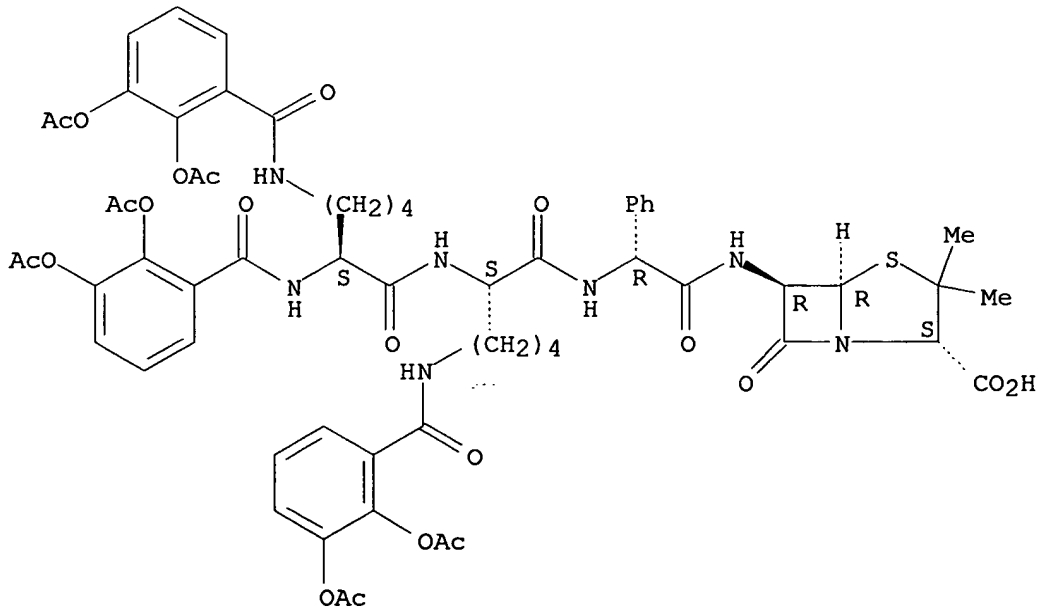


● Na

RN 454472-78-7 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N6-[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



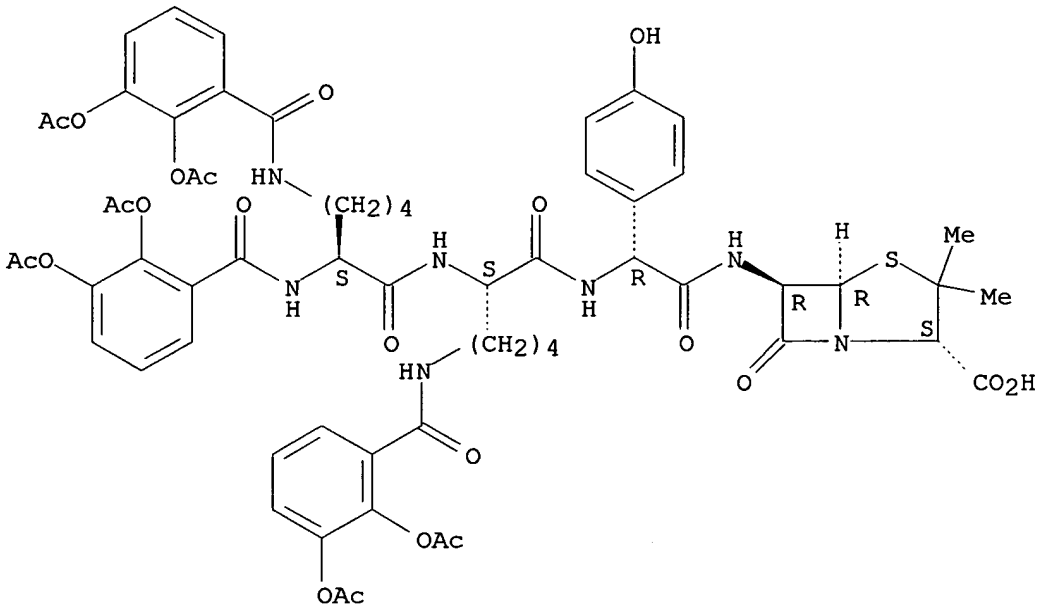
PAGE 2-A

● Na

RN 454472-79-8 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N6-[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-(4-hydroxyphenyl)-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



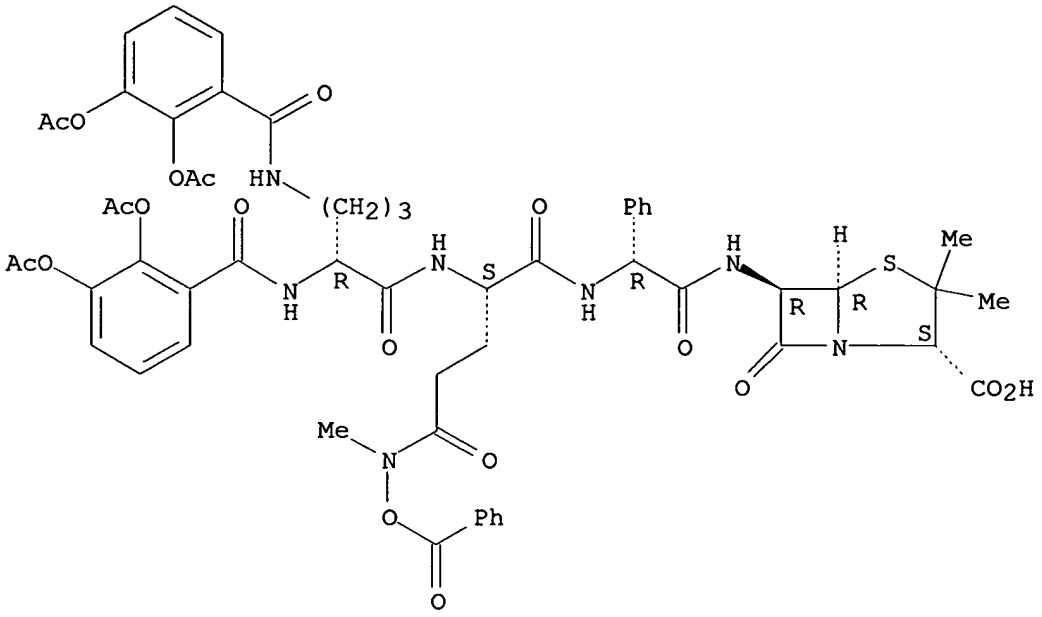
PAGE 2-A

● Na

RN 454472-80-1 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-D-ornithyl-N-(benzoyloxy)-N-methyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



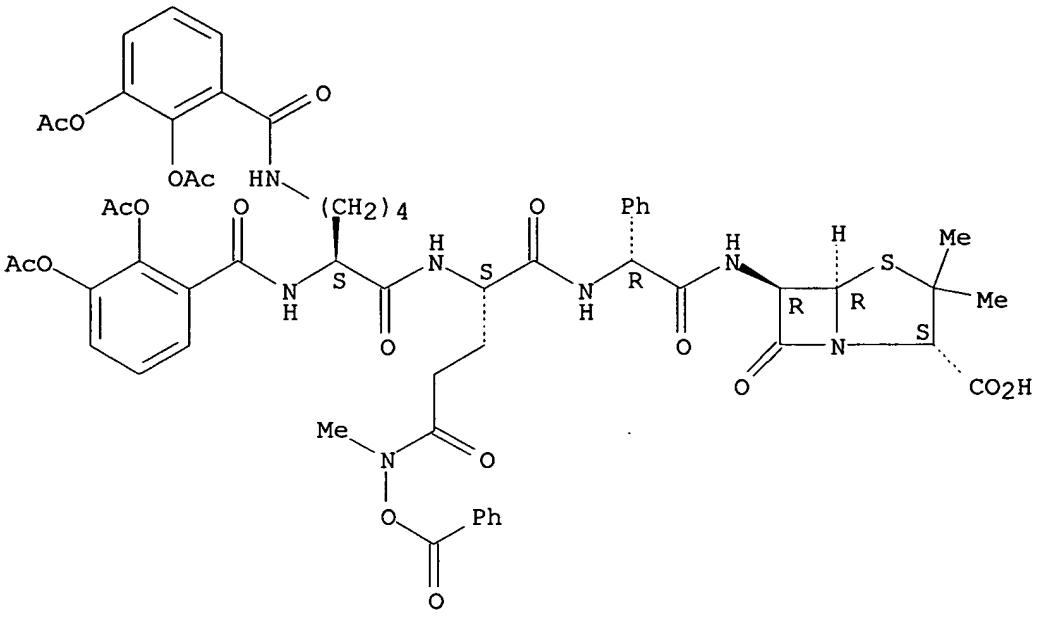
PAGE 2-A

● Na

RN 454472-81-2 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-(benzoyloxy)-N-methyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



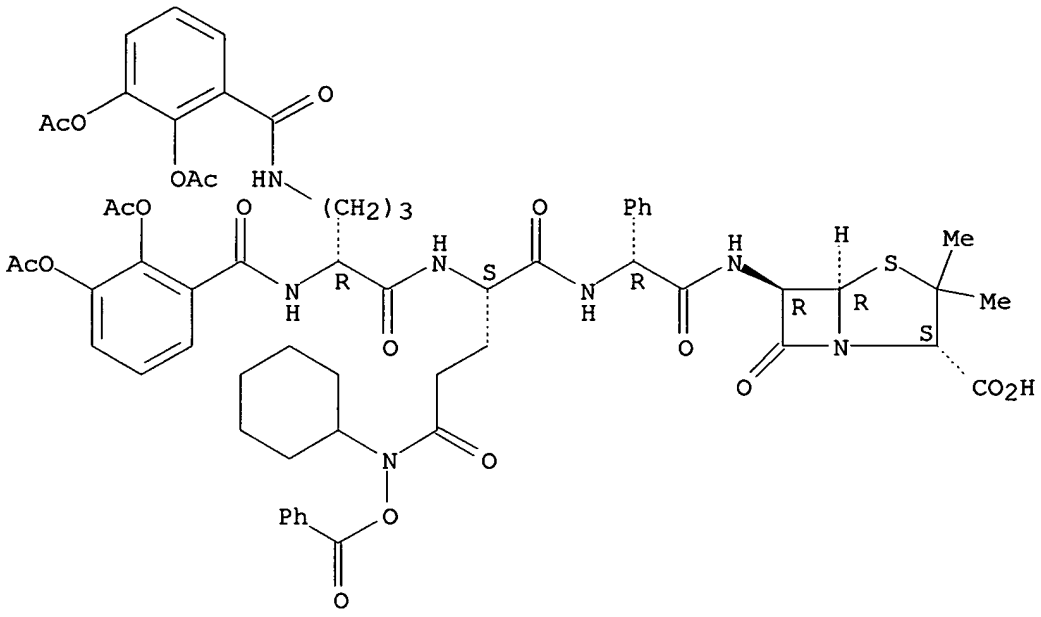
PAGE 2-A

● Na

RN 454472-82-3 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-D-ornithyl-N-(benzoyloxy)-N-cyclohexyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



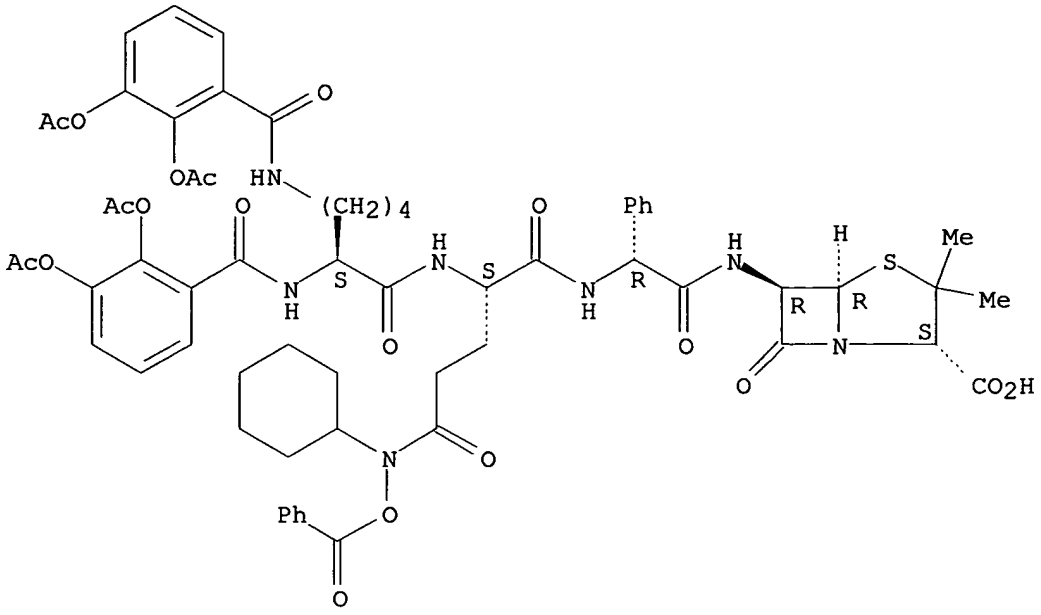
PAGE 2-A

● Na

RN 454472-87-8 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-(benzoyloxy)-N-cyclohexyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, monosodium salt, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

● Na

L27 ANSWER 3 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2002:615652 CAPLUS
DN 137:169797
TI Preparation of peptide derivatives as factor VIIa inhibitors
IN Shiraishi, Takuya; Kadono, Shojiro; Haramura, Masayuki; Sato, Haruhiko; Kozono, Toshiro; Koga, Takaki; Sakamoto, Akihisa
PA Chugai Seiyaku Kabushiki Kaisha, Japan
SO PCT Int. Appl., 246 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002062829	A1	20020815	WO 2002-JP883	20020204

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

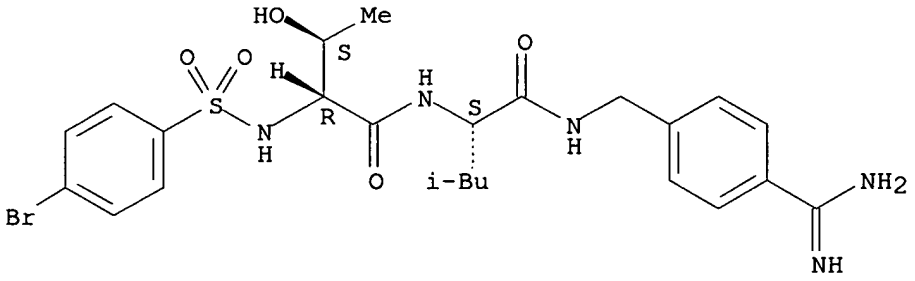
PRAI JP 2001-27474 A 20010202
OS MARPAT 137:169797
AB Dipeptide amide derivs. represented by the following general formula R1CH2NR2COCHR3NR4COCHR5NR6R7 [I; R1 = Q-Q6 (wherein R8 = NH2, aminomethyl, C(:NR9)NH2; R9 = H, NH2, OH, acyl, (un)substituted and linear or branched C1-6 alkoxy-carbonyl; one of X and Y is :CH and the other is N); R2 = H, linear or branched C1-6 alkyl; R3 = hydroxyphenyl, (CH2)mR11 (wherein R11 = CONH2, NR12CONH2, C(:NH)NH2; R12 = H, linear or branched C1-3 alkyl); R4 = H, linear or branched C1-6 alkyl; R7 = H, linear or branched C1-6 alkyl, SO2R14 (wherein R14 = linear or branched C1-8 alkyl)] are prepd. Crystals of a complex of VIIa factor/human sol. tissue factor with a low-mol. wt. reversible VIIa factor inhibitor selected from the dipeptide amide derivs. I are prepd. and studied by X-ray crystal structure anal. Also disclosed is a medium carrying the whole or a part of the coordinate data of the stereostructure of the complex of human VIIa factor/human sol. tissue factor with a low-mol. wt. reversible VIIa factor inhibitor obtained by X-ray crystal structure anal. of the above crystals recorded thereon. A method of designing a low-mol. wt. reversible VIIa factor inhibitor by using the above data is claimed. These peptide derivs. are useful as antithrombotics for preventing or treating deep venous thrombosis after surgery, restenosis after PTCA surgery, chronic thrombosis such as chronic DIC, cardiac thromboembolism, or myocardial or cerebral infarction. Thus, 1-(tert-butoxycarbonyl)-D-tryptophyl-N1-(4-cyanobenzyl)-L-glutamine (prepn. given) was condensed with 3-(methoxycarbonyl)benzylsulfonyl chloride in the presence of Et3N in DMF at room temp. for 12 h to give N-[[3-(methoxycarbonyl)benzyl]sulfonyl]-1-(tert-butoxycarbonyl)-D-tryptophyl-N1-(4-cyanobenzyl)-L-glutamine which was treated with satd. HCl/MeOH at room temp. for 20 h and refluxed with ammonium acetate and NH3 in ethanol for 1 h to give a mixt. of N-[[3-(methoxycarbonyl)benzyl]sulfonyl]-D-tryptophyl-N1-(4-amidinobenzyl)-L-glutamine and N-[[3-(ethoxycarbonyl)benzyl]sulfonyl]-D-tryptophyl-N1-(4-amidinobenzyl)-L-glutamine. The latter mixt. was stirred with a mixt. of ethanol and 2 N aq. EtOH at room temp. for 1 h and acidified with 1 N aq. HCl to give

N-[(3-carboxybenzyl)sulfonyl]-D-tryptophyl-N1-(4-amidinobenzyl)-L-glutamine (II). II in vitro inhibited factor VIIa and thrombin with IC50 of 37 and 17,870 nM, resp. A complex of human factor VII/human sol. tissue factor with N-(carboxymethylsulfonyl)-D-tryptophyl-N1-(4-amidinobenzyl)-L-glutamine and that with N-(ethanesulfonyl)-p-phenyl-D-phenylalanyl-N1-(4-amidinobenzyl)-L-glutamine were prepd. in a cryst. form and studied by X-ray crystal structure anal.

IT **446846-00-0P 446846-01-1P 446846-03-3P**
446846-04-4P 446846-19-1P 446846-24-8P
446846-25-9P 446846-26-0P 446846-27-1P
446846-54-4P 446846-55-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of peptide derivs. as VIIa factor inhibitors and antithrombotics and X-ray crystal structure anal. of human VIIa factor-peptide inhibitor complex)

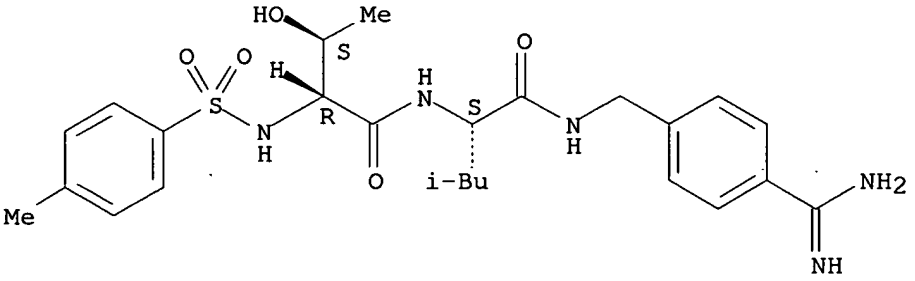
RN 446846-00-0 CAPLUS
CN L-Leucinamide, N-[(4-bromophenyl)sulfonyl]-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



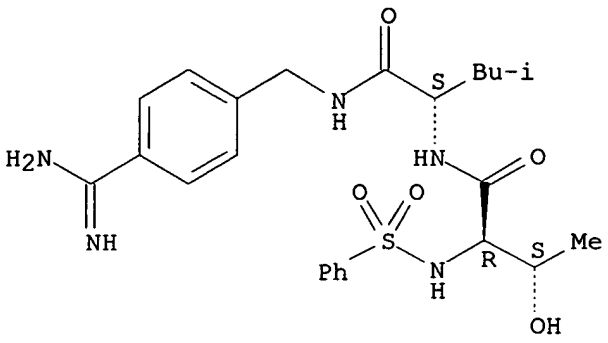
RN 446846-01-1 CAPLUS
CN L-Leucinamide, N-[(4-methylphenyl)sulfonyl]-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



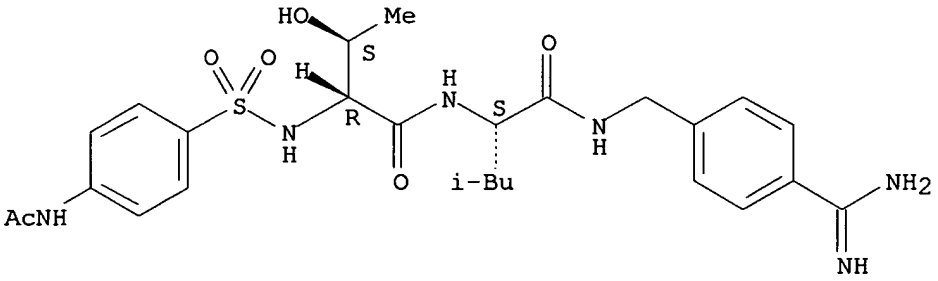
RN 446846-03-3 CAPLUS
CN L-Leucinamide, N-(phenylsulfonyl)-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



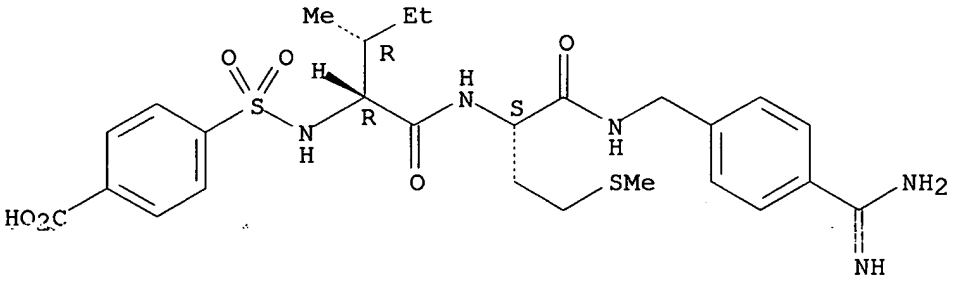
RN 446846-04-4 CAPLUS
CN L-Leucinamide, N-[[4-(acetylamino)phenyl]sulfonyl]-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



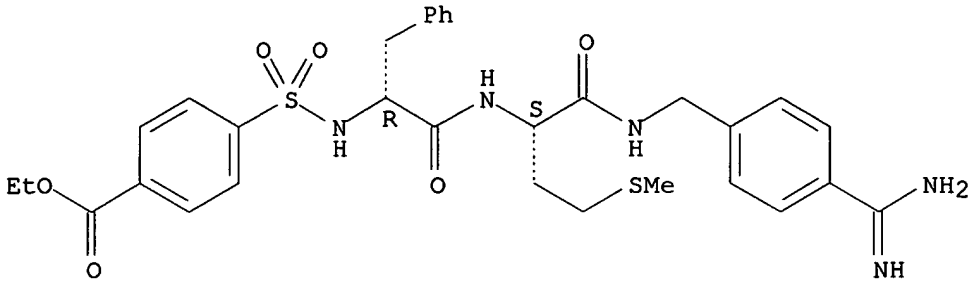
RN 446846-19-1 CAPLUS
CN L-Methioninamide, N-[(4-carboxyphenyl)sulfonyl]-D-isoleucyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



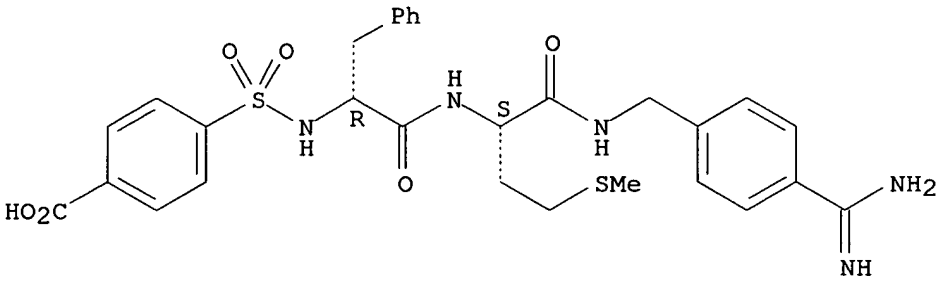
RN 446846-24-8 CAPLUS
CN L-Methioninamide, N-[[4-(ethoxycarbonyl)phenyl]sulfonyl]-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



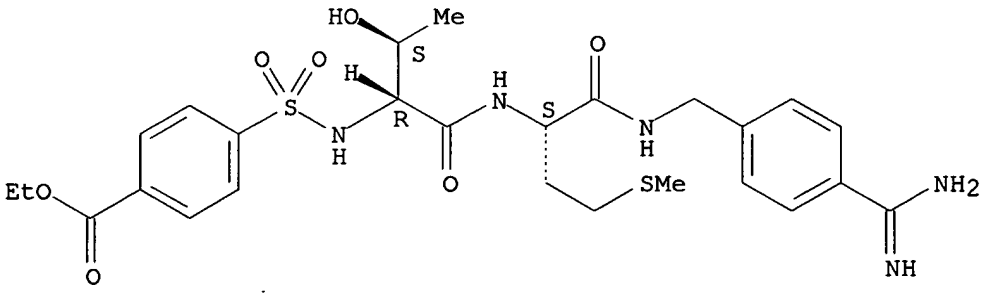
RN 446846-25-9 CAPLUS
CN L-Methioninamide, N-[(4-carboxyphenyl)sulfonyl]-D-phenylalanyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



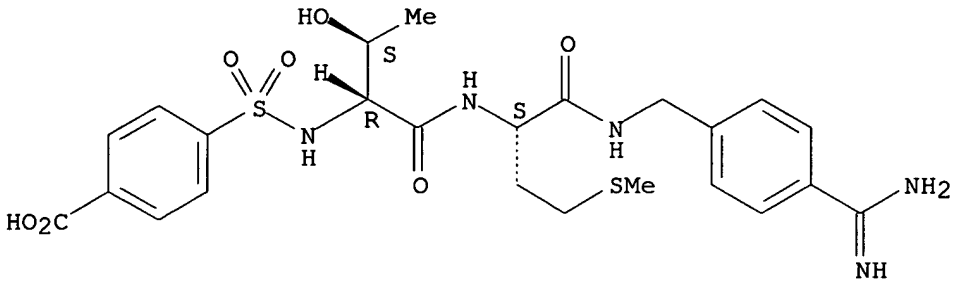
RN 446846-26-0 CAPLUS
CN L-Methioninamide, N-[[4-(ethoxycarbonyl)phenyl]sulfonyl]-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



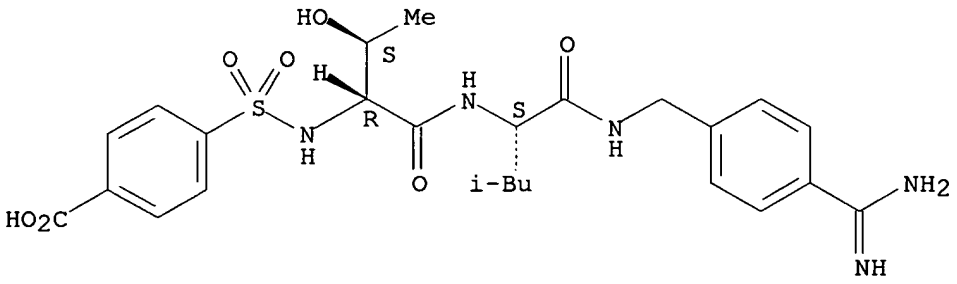
RN 446846-27-1 CAPLUS
CN L-Methioninamide, N-[(4-carboxyphenyl)sulfonyl]-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



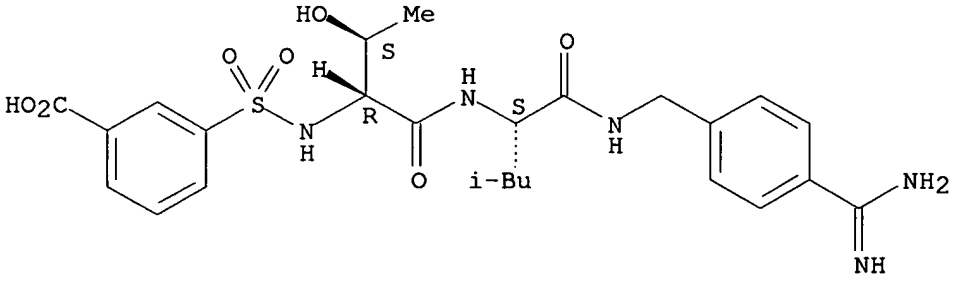
RN 446846-54-4 CAPLUS
CN L-Leucinamide, N-[(4-carboxyphenyl)sulfonyl]-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 446846-55-5 CAPLUS
CN L-Leucinamide, N-[(3-carboxyphenyl)sulfonyl]-D-threonyl-N-[[4-(aminoiminomethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 4 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2002:487516 CAPLUS
DN 137:63474
TI Preparation of amino acid-related diamines as modulators of chemokine receptor activity
IN Carter, Percy; Cherney, Robert
PA Bristol-Myers Squibb Pharma Co., USA
SO PCT Int. Appl., 375 pp.
CODEN: PIXXD2
DT Patent
LA English

Appl. PCT

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002050019	A2	20020627	WO 2001-US50619	20011220
	WO 2002050019	A3	20030313		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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	AU 2002041724	A5	20020701	AU 2002-41724	20011220
	US 2003060459	A1	20030327	US 2001-27505	20011220
PRAI	US 2000-256855P	P	20001220		
	WO 2001-US50619	W	20011220		

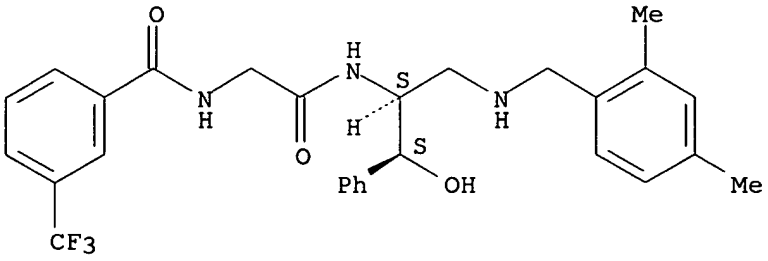
OS MARPAT 137:63474

AB Diamine compds. R1-X-CR6R7(CR8R9)m(CR10R11)lCR12R3NHCO(CR14R14a)nNR15-Z-R2 [Z = a bond, CONH, C(S)NH, SO2, SO2NH; X = NH, (cyclo)alkylimino, O, S, methyleneimino optionally substituted by (cyclo)alkyl; R1, R2 = (hetero)aryl; R3 = H, functionalized alkyl, (hetero)cyclyl; R6-R12 = alkyl, alkenyl, alkynyl, any group given for R3; R14, R14a = (un)substituted alkyl; n = 1 or 2; l, m = 0 or 1] or their pharmaceutically acceptable salt were prepd. as modulators of chemokine receptor activity for use in the treatment and prevention of asthma, multiple sclerosis, atherosclerosis, and rheumatoid arthritis. One hundred ninety-four diamines, e.g., Me (2S)-3-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]propanoate, were synthesized and claimed. All examples of the present invention have activity (IC50 = 50% at .ltorsim. 20 .mu.M) in the antagonism of MCP-1 binding to human PBMC (human peripheral blood mononuclear cells).

IT **439149-10-7P 439149-11-8P**
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)

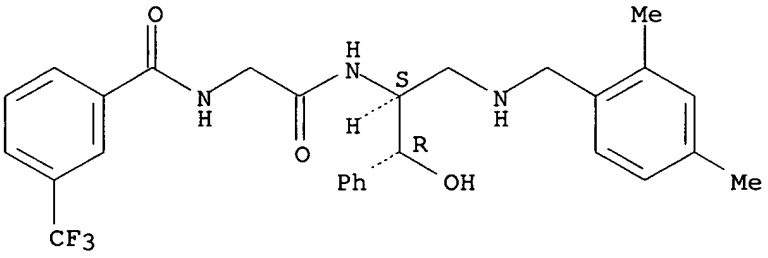
RN 439149-10-7 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



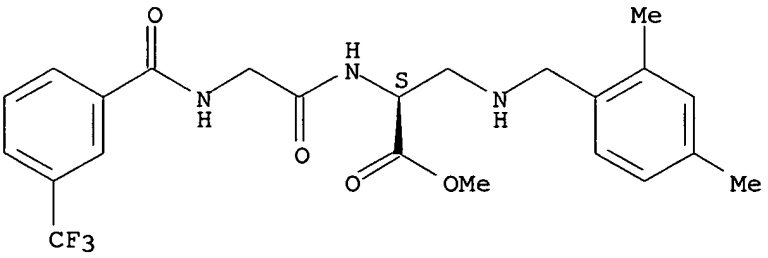
RN 439149-11-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



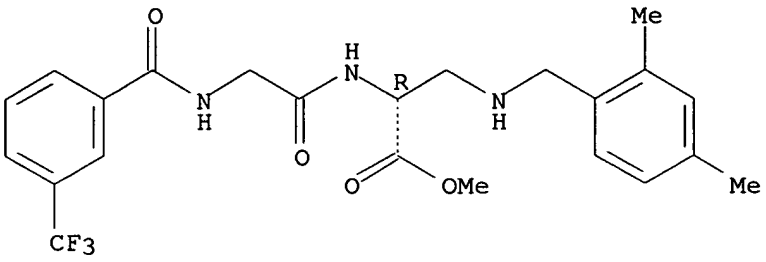
IT **439148-61-5P 439148-62-6P 439148-63-7P**
439148-76-2P 439148-85-3P 439148-98-8P
439149-02-7P 439149-18-5P 439149-47-0P
439150-06-8P 439150-30-8P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)
RN 439148-61-5 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



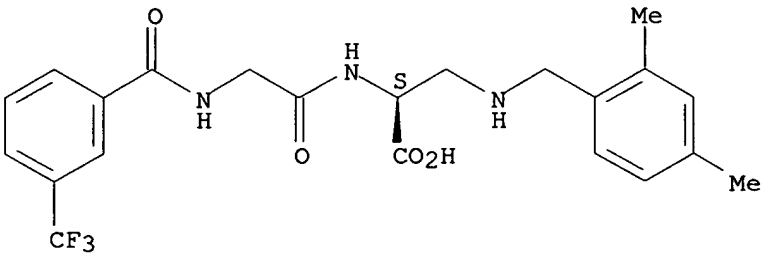
RN 439148-62-6 CAPLUS
CN D-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



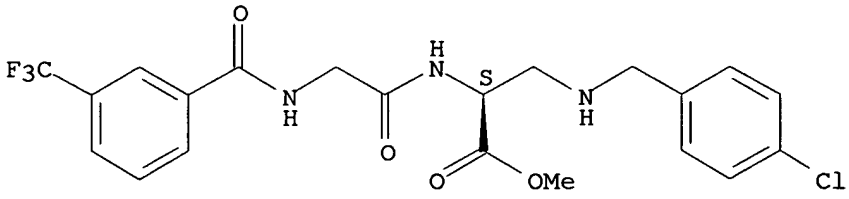
RN 439148-63-7 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



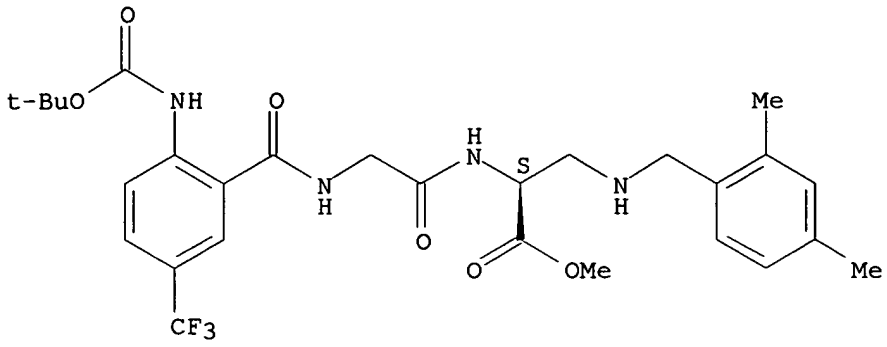
RN 439148-76-2 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-chlorophenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



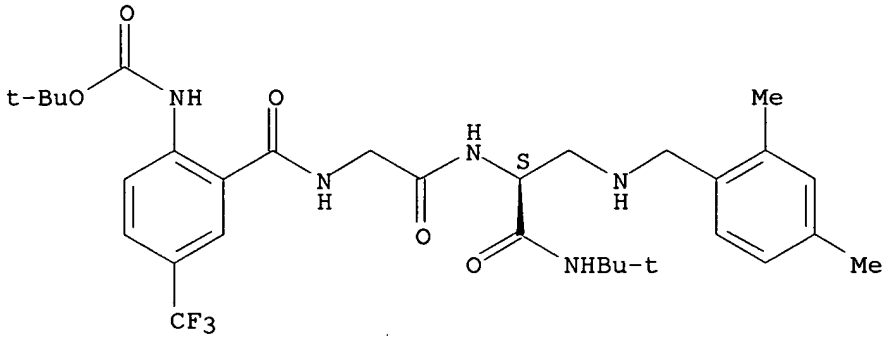
RN 439148-85-3 CAPLUS
CN L-Alanine, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



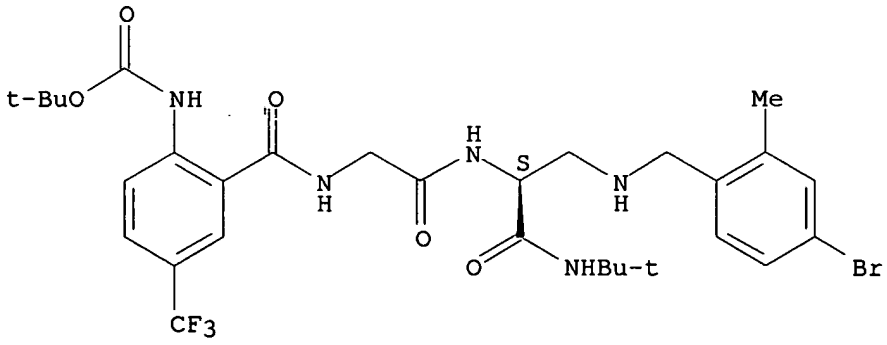
RN 439148-98-8 CAPLUS
CN L-Alaninamide, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439149-02-7 CAPLUS
CN L-Alaninamide, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

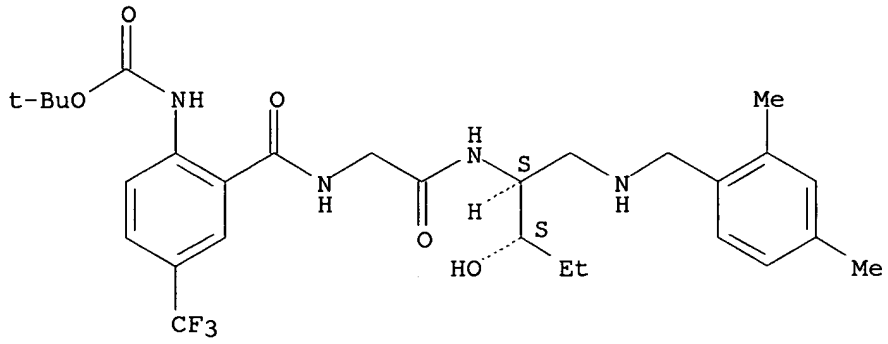
Absolute stereochemistry.



RN 439149-18-5 CAPLUS

CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-1-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

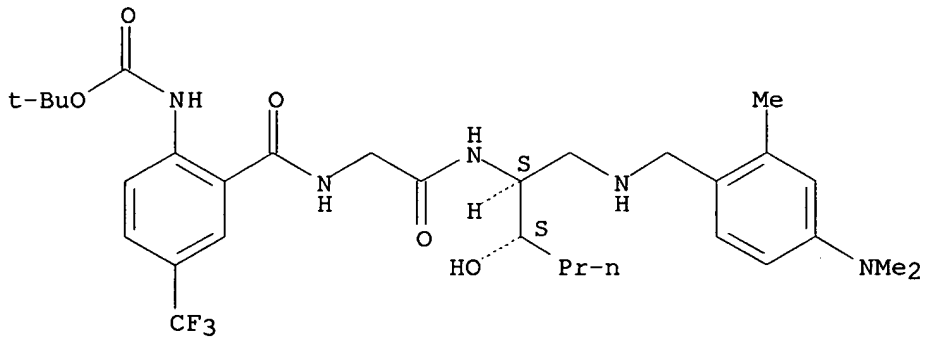
Absolute stereochemistry.



RN 439149-47-0 CAPLUS

CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[[4-(dimethylamino)-2-methylphenyl]methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

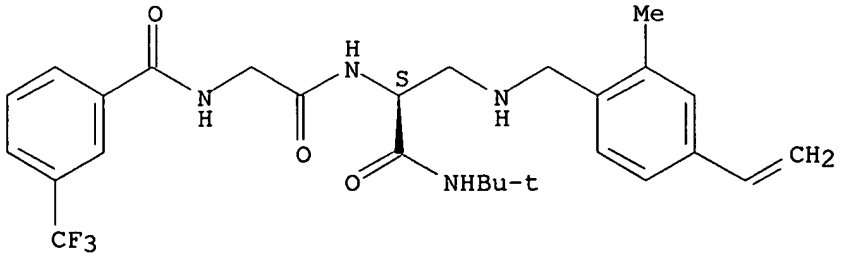
Absolute stereochemistry.



RN 439150-06-8 CAPLUS

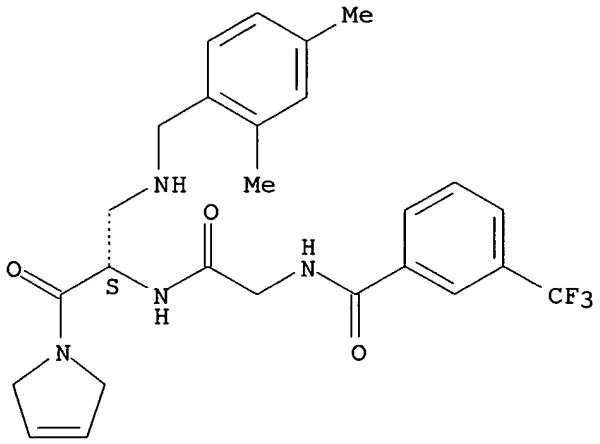
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-ethenyl-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439150-30-8 CAPLUS
CN Benzamide, N-[2-[[(1S)-2-(2,5-dihydro-1H-pyrrol-1-yl)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-oxoethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **439148-64-8P 439148-65-9P 439148-66-0P**
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439148-89-7P 439148-91-1P 439148-94-4P
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439149-69-6P 439149-70-9P 439149-71-0P
439149-72-1P 439149-73-2P 439149-74-3P
439149-75-4P 439149-76-5P 439149-77-6P
439149-78-7P 439149-79-8P 439149-80-1P
439149-81-2P 439149-82-3P 439149-83-4P
439149-84-5P 439149-85-6P 439149-86-7P

439149-87-8P 439149-88-9P 439149-89-0P
439149-90-3P 439149-91-4P 439149-92-5P
439149-93-6P 439149-94-7P 439149-95-8P
439149-96-9P 439149-97-0P 439149-98-1P
439149-99-2P 439150-00-2P 439150-01-3P
439150-03-5P 439150-04-6P 439150-05-7P
439150-07-9P 439150-08-0P 439150-09-1P
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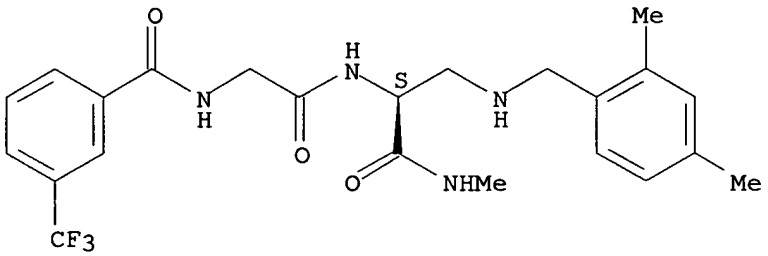
439150-13-7P 439150-14-8P 439150-15-9P
439150-17-1P 439150-18-2P 439150-19-3P
439150-20-6P 439150-21-7P 439150-22-8P
439150-23-9P 439150-24-0P 439150-25-1P
439150-26-2P 439150-27-3P 439150-28-4P
439150-29-5P 439150-31-9P 439150-32-0P
439150-33-1P 439150-34-2P 439150-35-3P
439150-36-4P 439150-37-5P 439150-53-5P
439150-54-6P 439150-55-7P 439150-56-8P
439150-57-9P 439150-58-0P 439150-65-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)

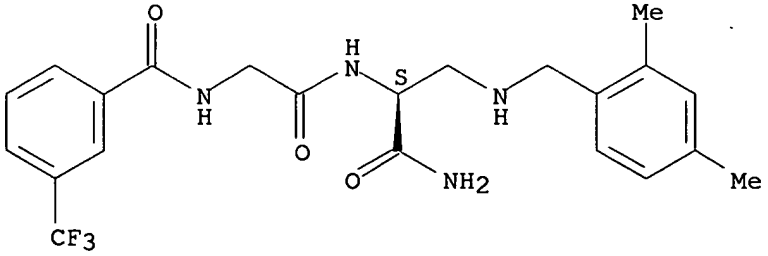
RN 439148-64-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439148-65-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

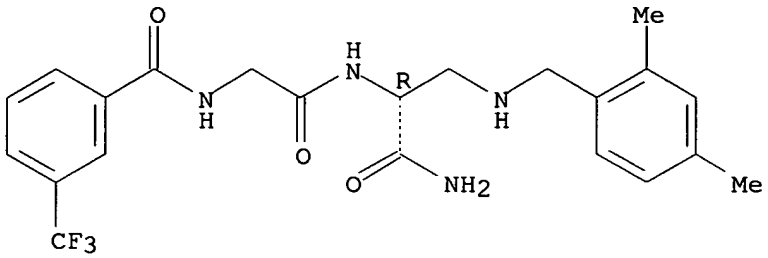
Absolute stereochemistry.



RN 439148-66-0 CAPLUS

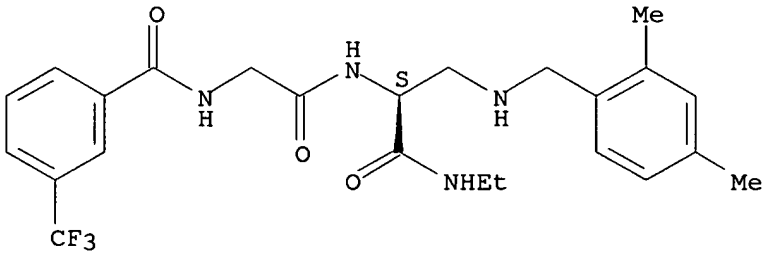
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



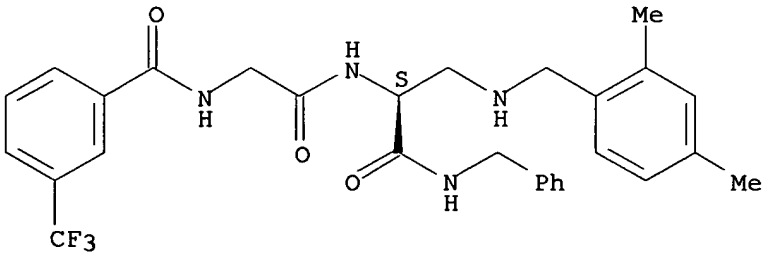
RN 439148-67-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



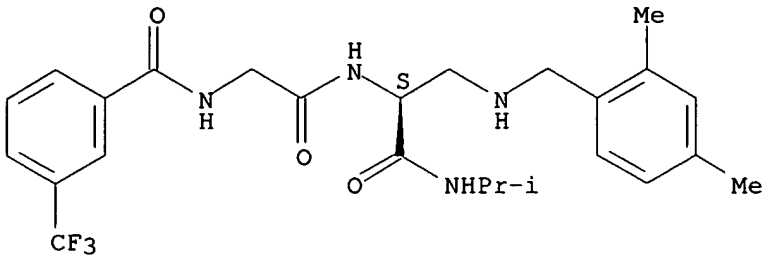
RN 439148-68-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



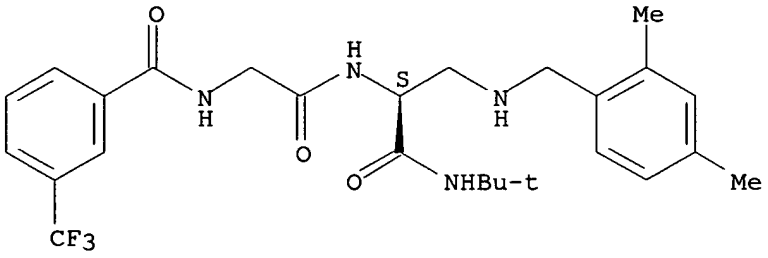
RN 439148-69-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



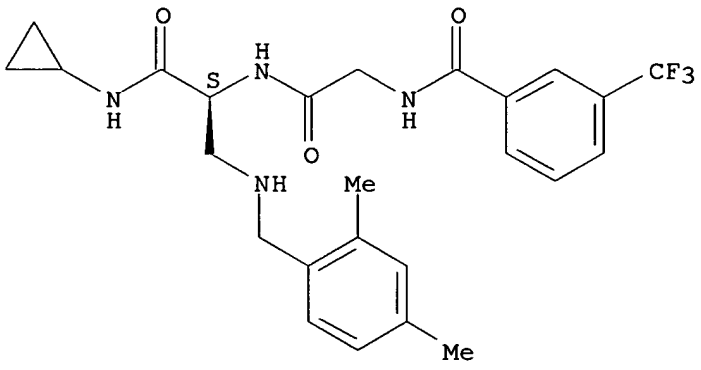
RN 439148-70-6 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



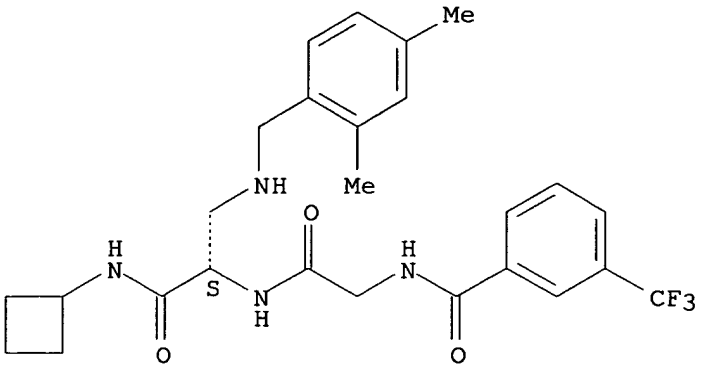
RN 439148-71-7 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclopropyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



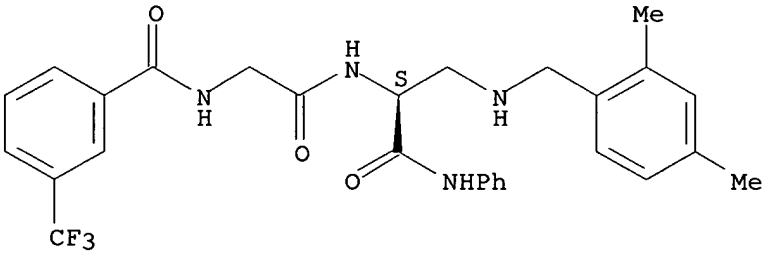
RN 439148-72-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclobutyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



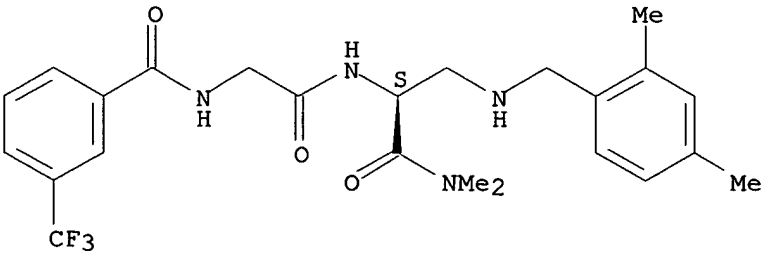
RN 439148-73-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



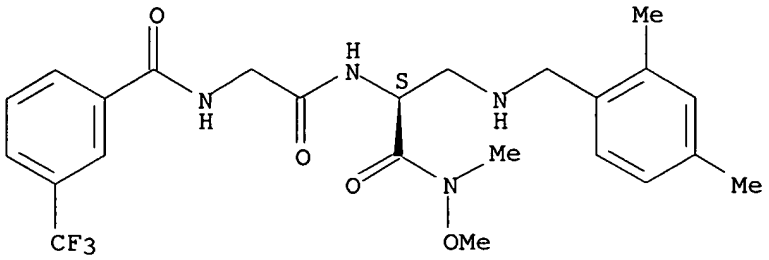
RN 439148-74-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N,N-dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



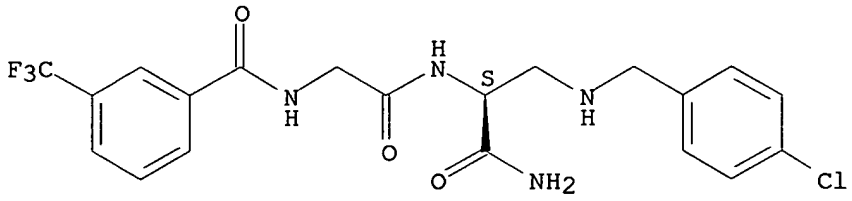
RN 439148-75-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-methoxy-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



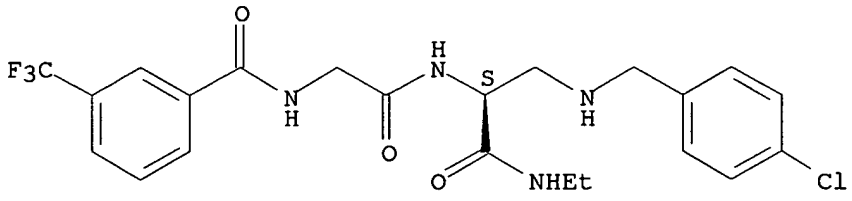
RN 439148-77-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-chlorophenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



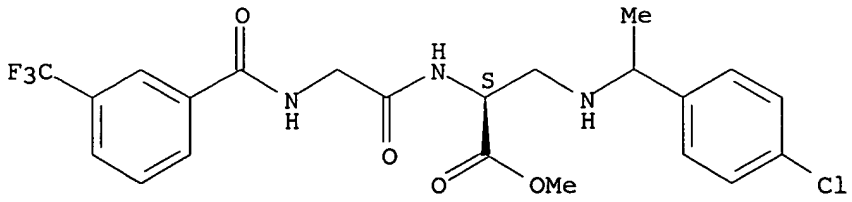
RN 439148-78-4 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-chlorophenyl)methyl]amino]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439148-79-5 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[1-(4-chlorophenyl)ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

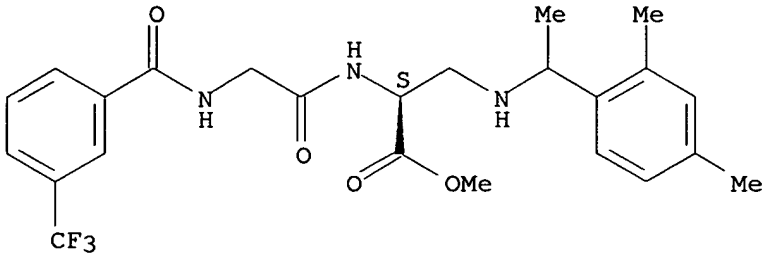
Absolute stereochemistry.



RN 439148-80-8 CAPLUS

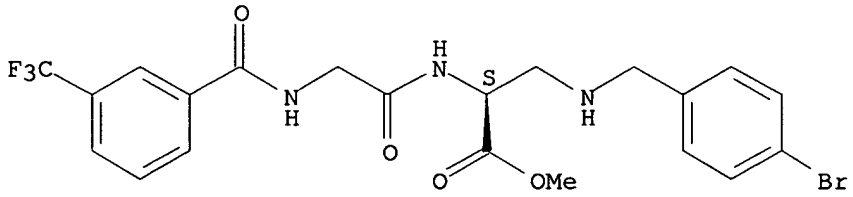
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[1-(2,4-dimethylphenyl)ethyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



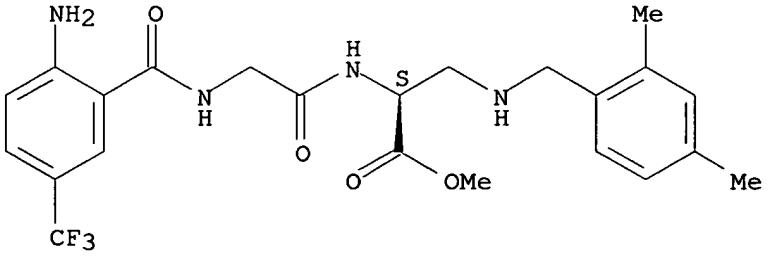
RN 439148-84-2 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromophenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



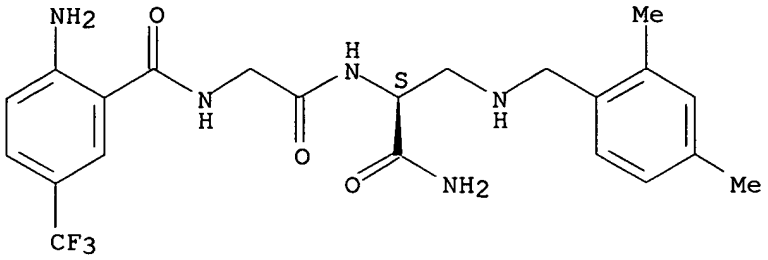
RN 439148-86-4 CAPLUS
CN L-Alanine, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



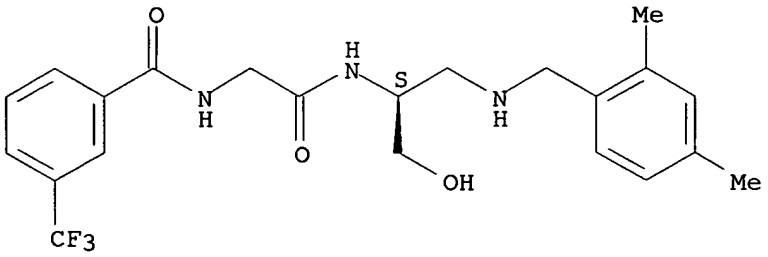
RN 439148-89-7 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



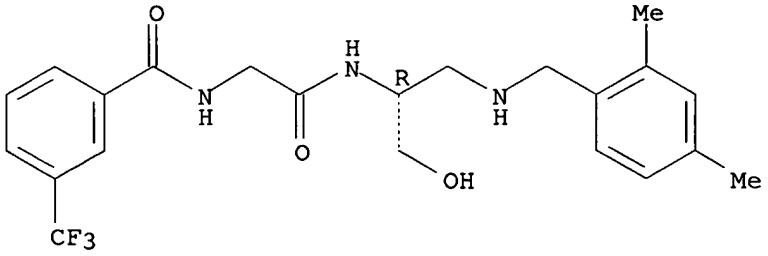
RN 439148-91-1 CAPLUS
CN Benzamide, N-[2-[[(1S)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-(hydroxymethyl)ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



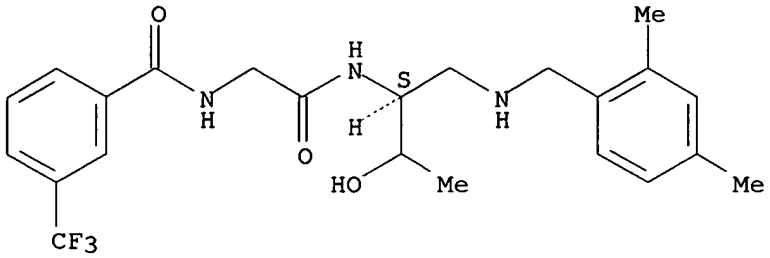
RN 439148-94-4 CAPLUS
CN Benzamide, N-[2-[[(1R)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-(hydroxymethyl)ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



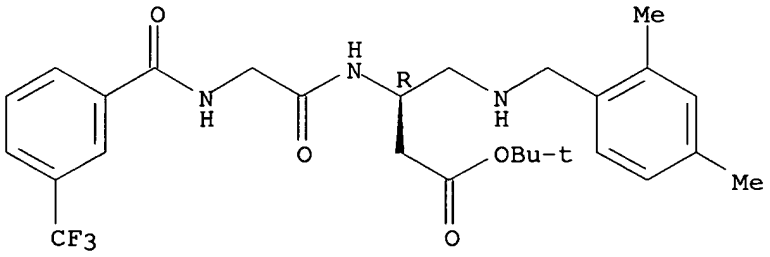
RN 439148-95-5 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



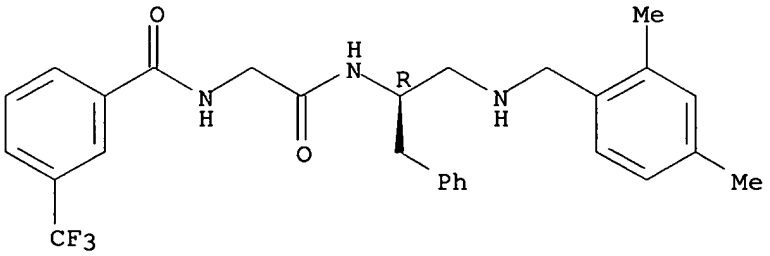
RN 439148-96-6 CAPLUS
CN Butanoic acid, 4-[[(2,4-dimethylphenyl)methyl]amino]-3-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



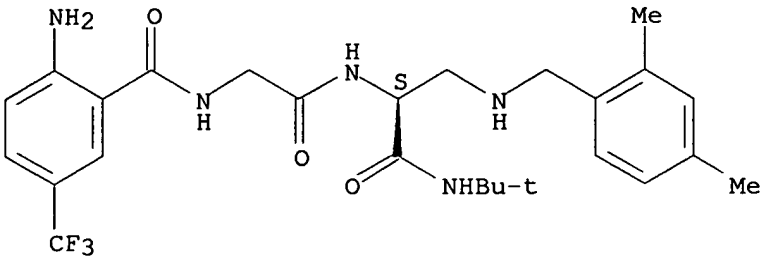
RN 439148-97-7 CAPLUS
CN Benzamide, N-[2-[[(1R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



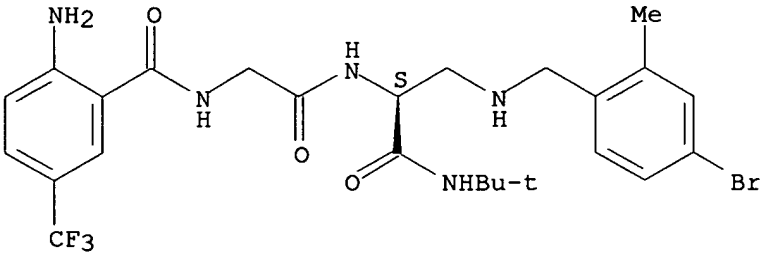
RN 439149-00-5 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



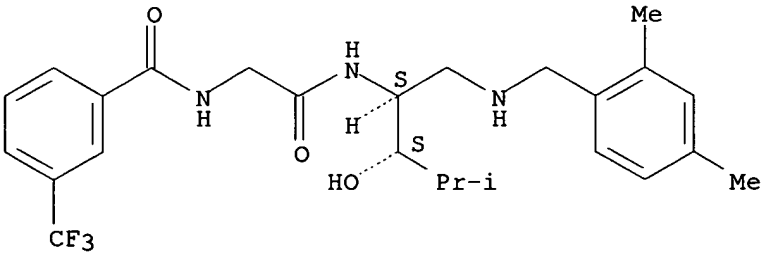
RN 439149-04-9 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



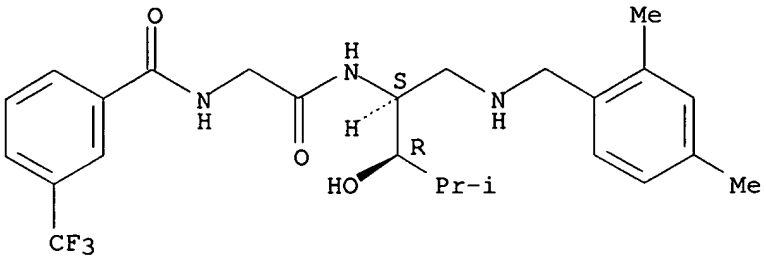
RN 439149-06-1 CAPLUS
CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



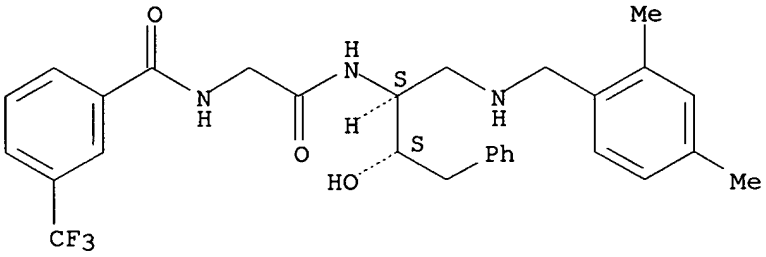
RN 439149-09-4 CAPLUS
CN D-erythro-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



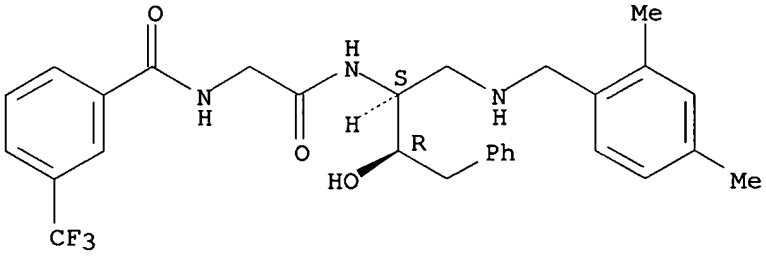
RN 439149-12-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-3-phenylpropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



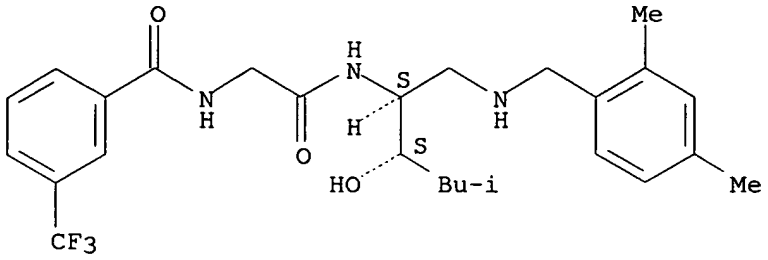
RN 439149-13-0 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-3-phenylpropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



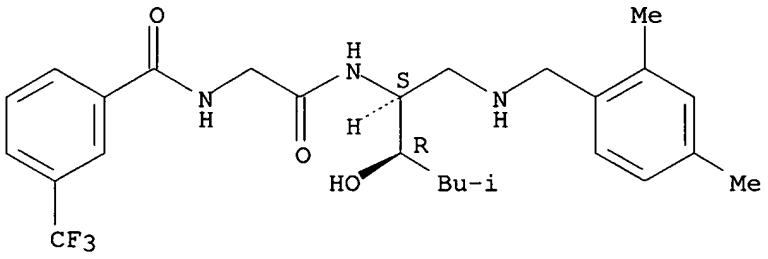
RN 439149-14-1 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



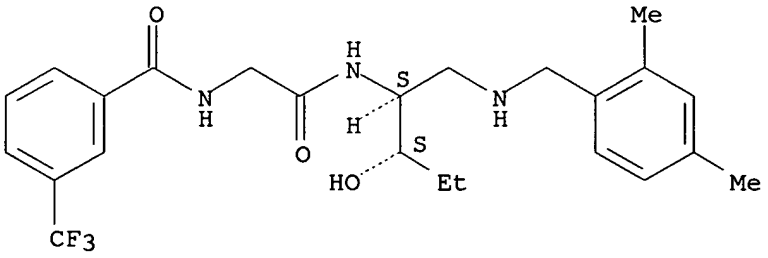
RN 439149-15-2 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



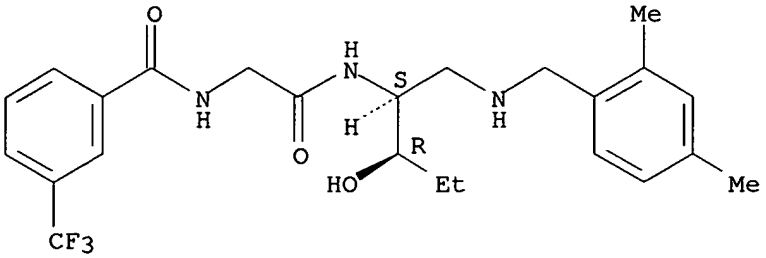
RN 439149-16-3 CAPLUS
CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



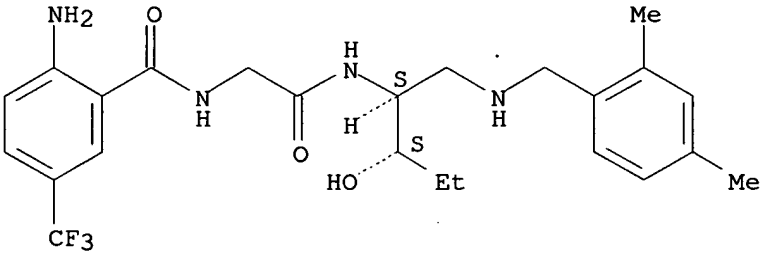
RN 439149-17-4 CAPLUS
CN D-erythro-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



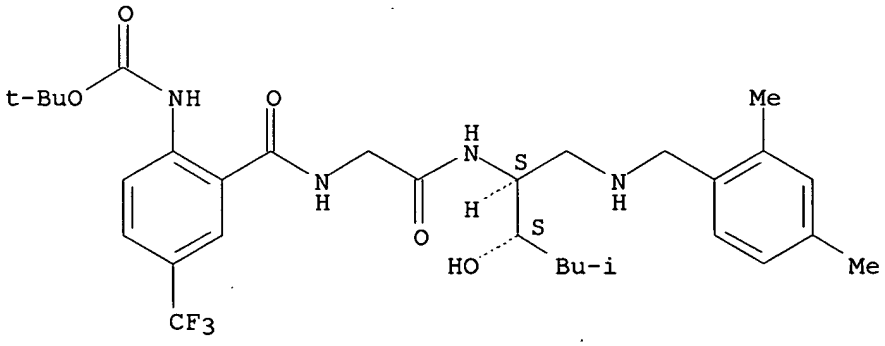
RN 439149-19-6 CAPLUS
CN D-erythro-Pentitol, 2-[[[[2-amino-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



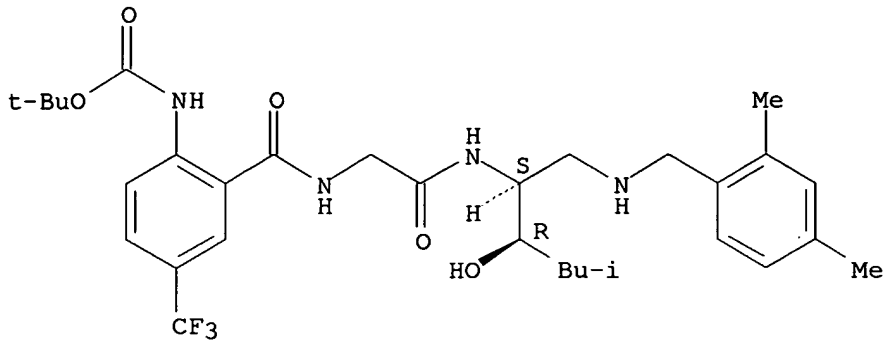
RN 439149-20-9 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



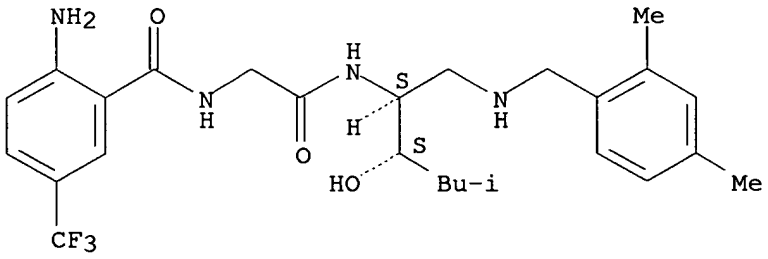
RN 439149-21-0 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



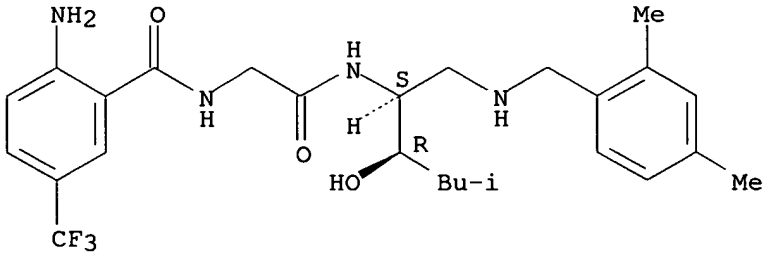
RN 439149-22-1 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



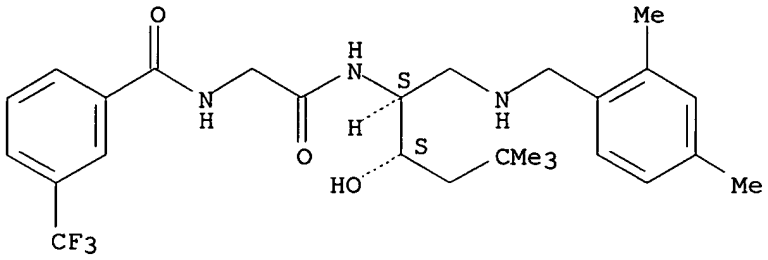
RN 439149-23-2 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



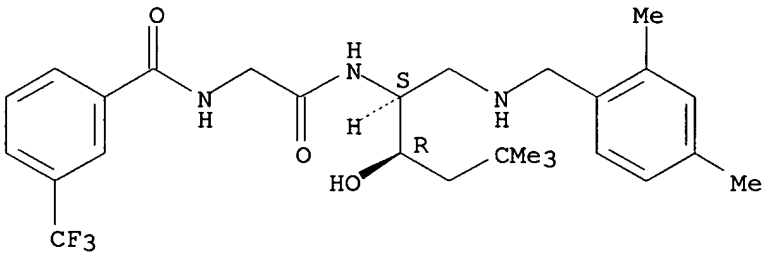
RN 439149-24-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4,4-dimethylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



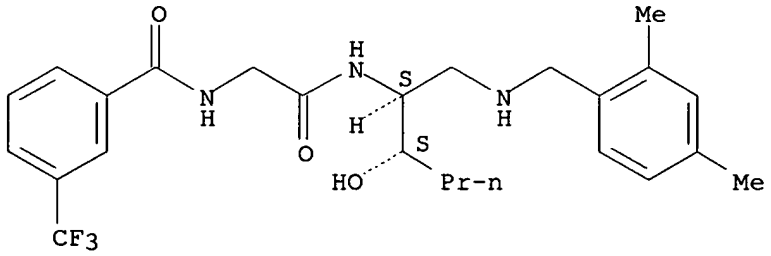
RN 439149-25-4 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4,4-dimethylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



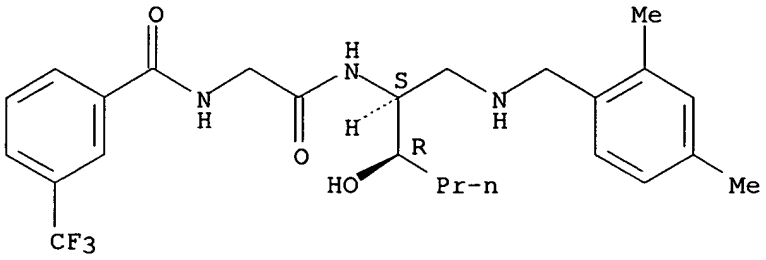
RN 439149-26-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



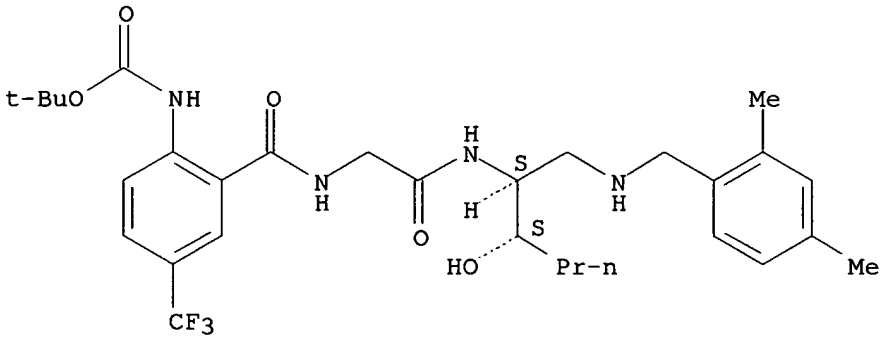
RN 439149-27-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



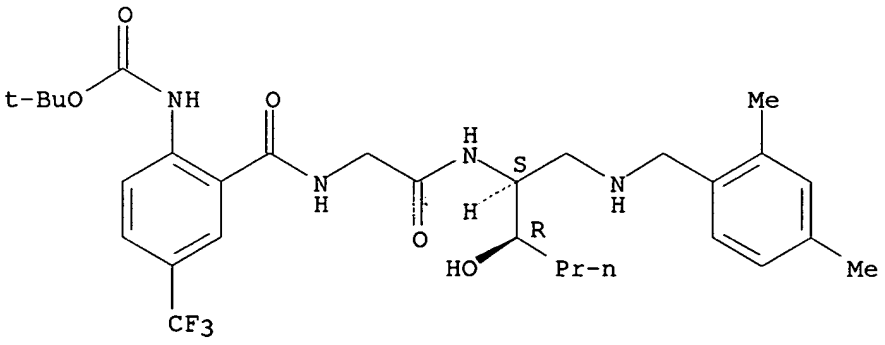
RN 439149-28-7 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



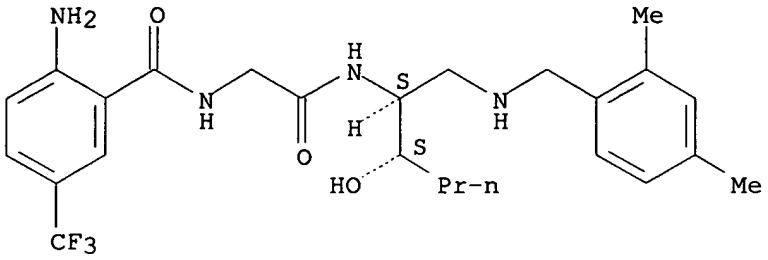
RN 439149-29-8 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439149-30-1 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

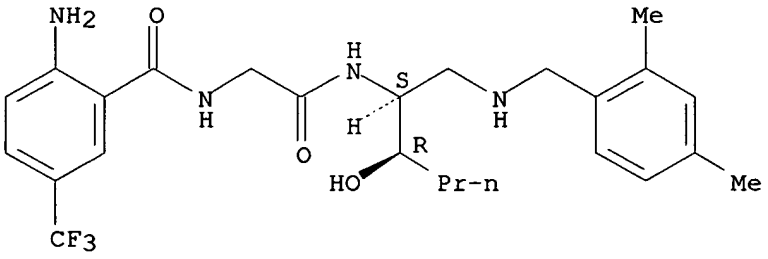
Absolute stereochemistry.



Elected species.

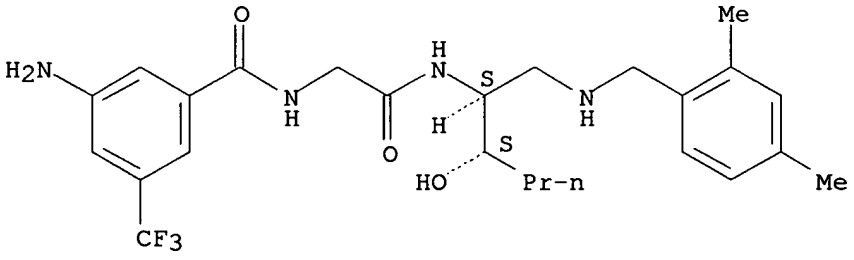
RN 439149-31-2 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



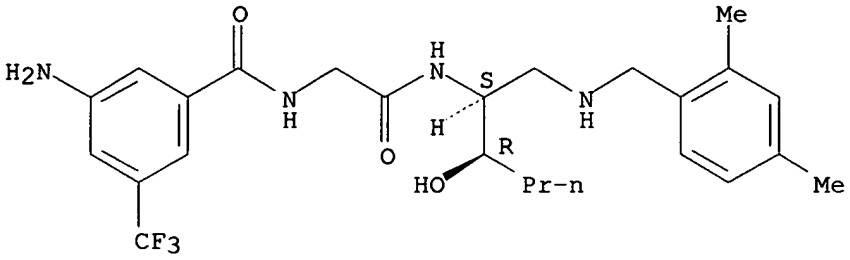
RN 439149-32-3 CAPLUS
CN Benzamide, 3-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



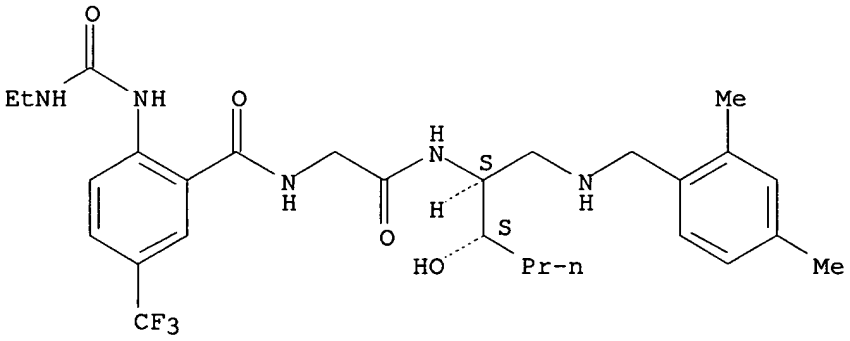
RN 439149-33-4 CAPLUS
CN Benzamide, 3-amino-N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



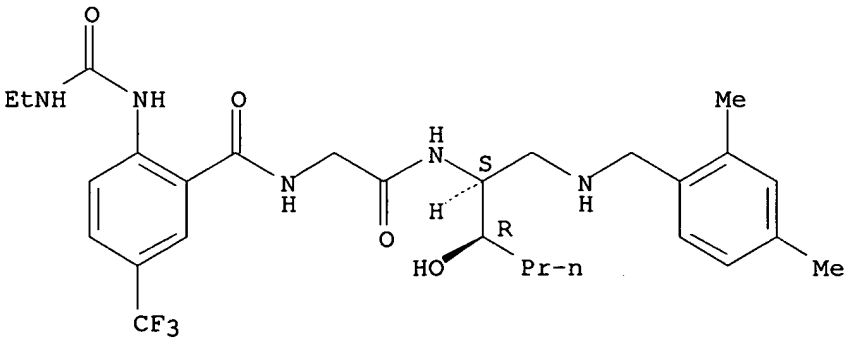
RN 439149-34-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[(ethylamino)carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



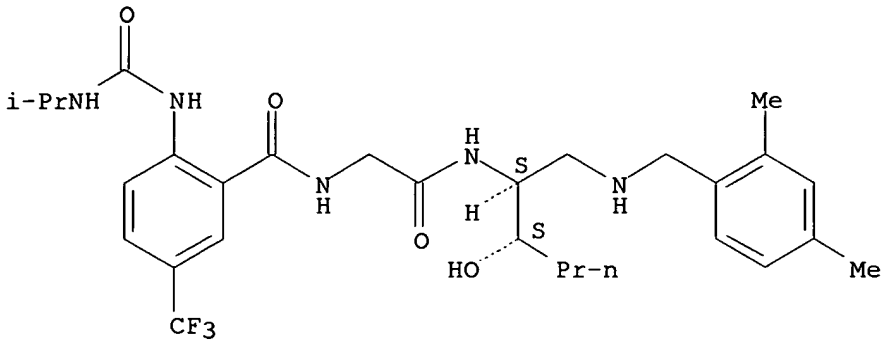
RN 439149-35-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[(ethylamino)carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



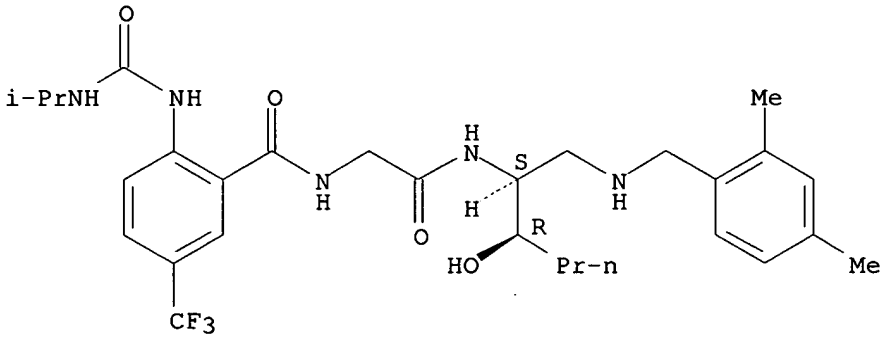
RN 439149-36-7 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



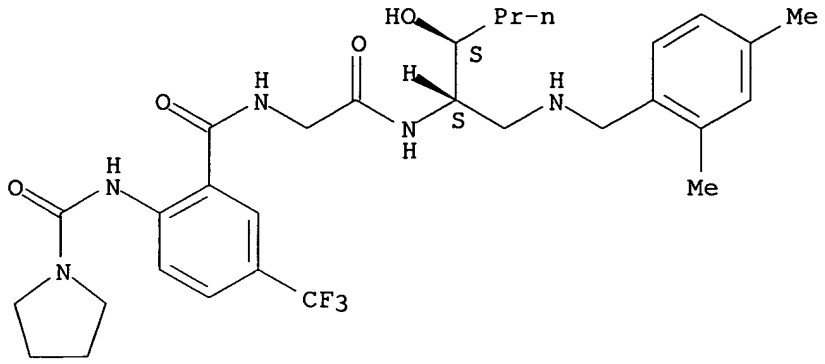
RN 439149-37-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



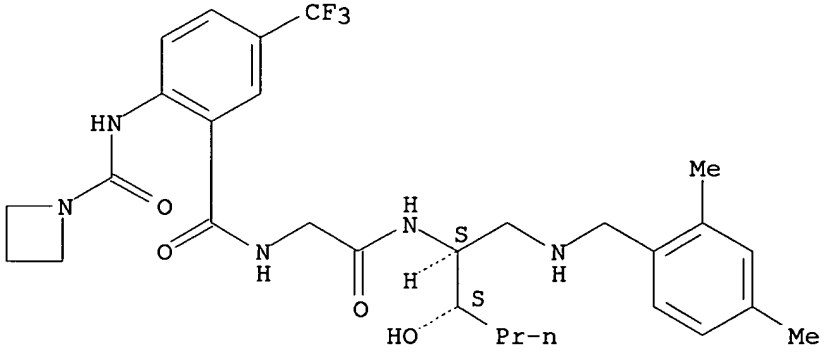
RN 439149-38-9 CAPLUS
CN 1-Pyrrolidinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



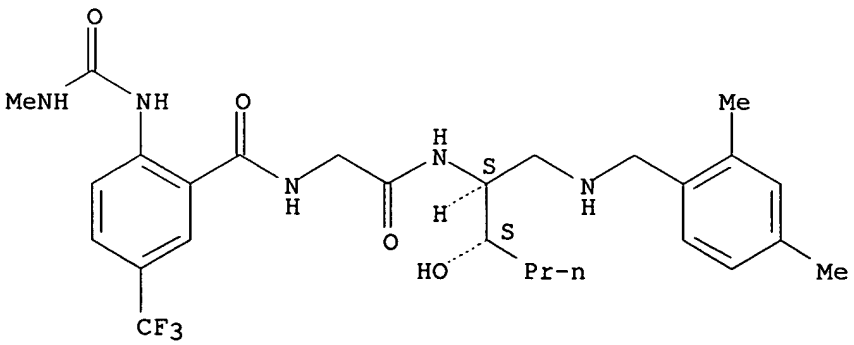
RN 439149-39-0 CAPLUS
CN 1-Azetidinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



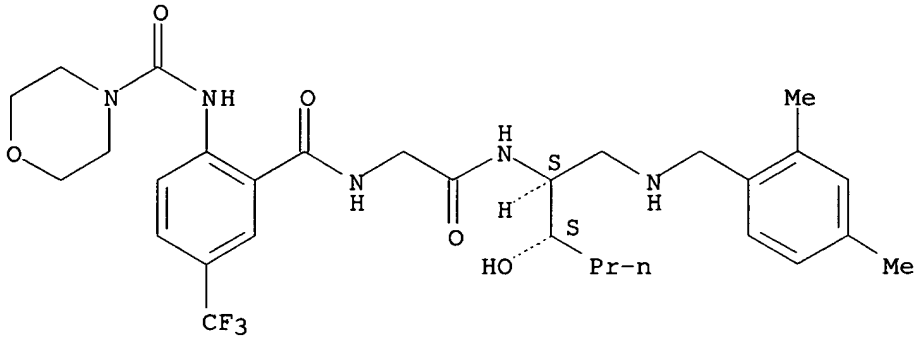
RN 439149-40-3 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[(methylamino)carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



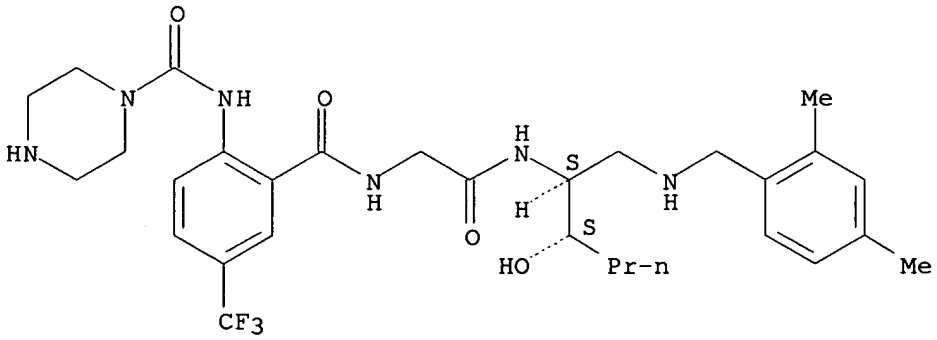
RN 439149-41-4 CAPLUS
CN 4-Morpholinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



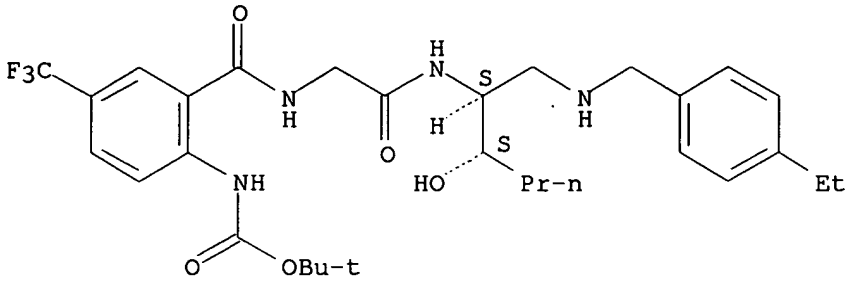
RN 439149-42-5 CAPLUS
CN 1-Piperazinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



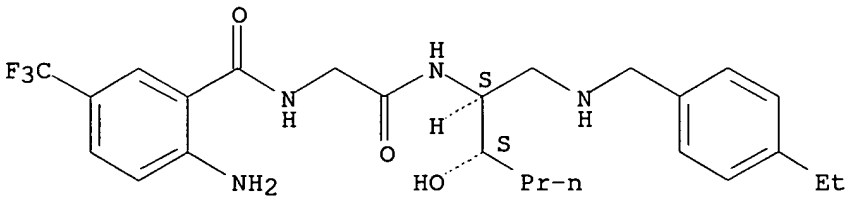
RN 439149-43-6 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



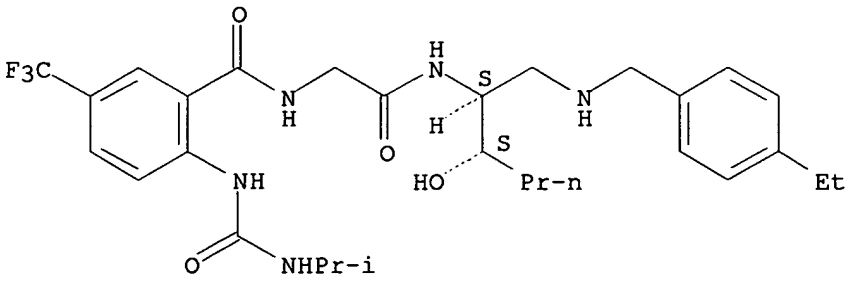
RN 439149-44-7 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



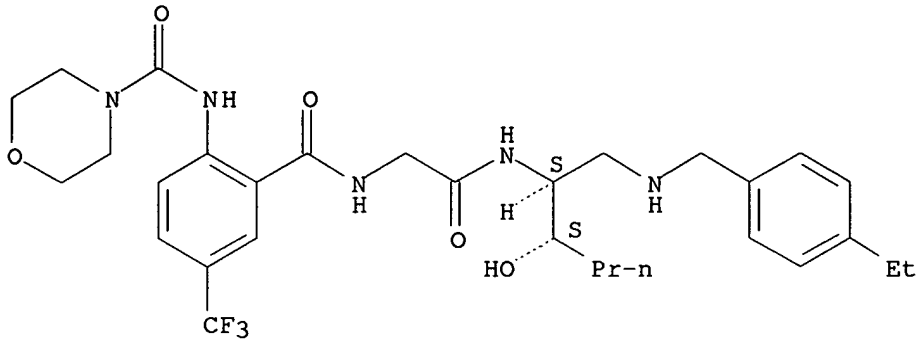
RN 439149-45-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



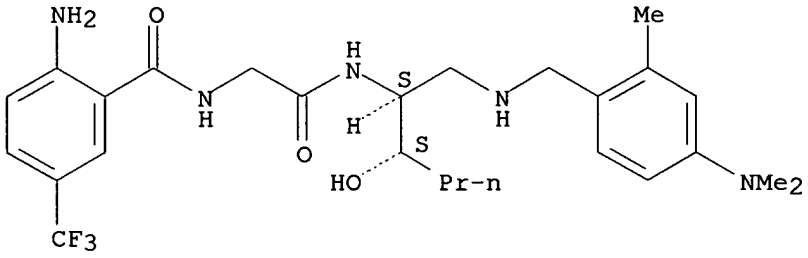
RN 439149-46-9 CAPLUS
CN 4-Morpholinecarboxamide, N-[2-[[[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



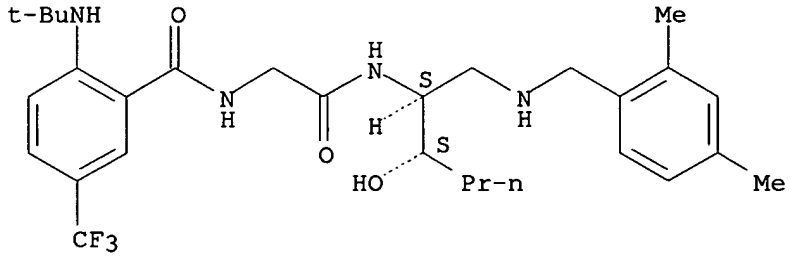
RN 439149-48-1 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[[4-(dimethylamino)-2-methylphenyl]methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



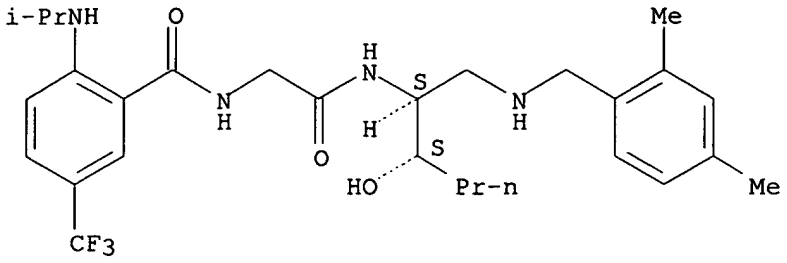
RN 439149-49-2 CAPLUS
CN Benzamide, 2-[(1,1-dimethylethyl)amino]-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



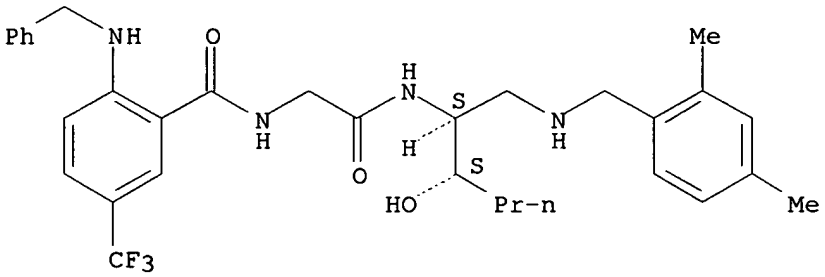
RN 439149-50-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[(1-methylethyl)amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



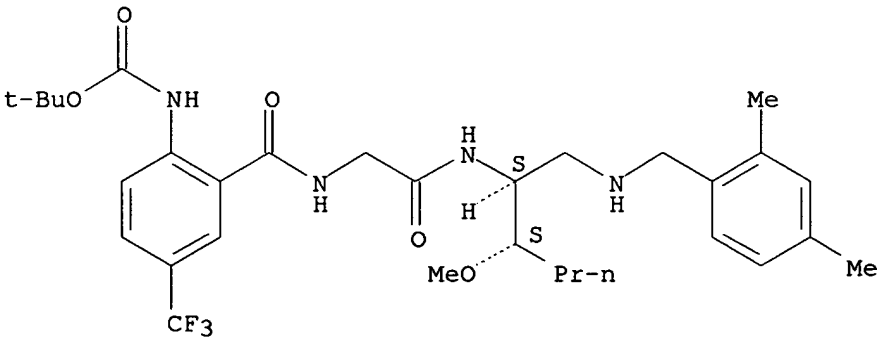
RN 439149-51-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[(phenylmethyl)amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



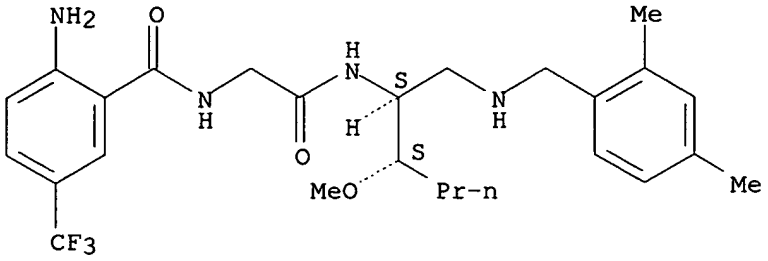
RN 439149-52-7 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-methoxypentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



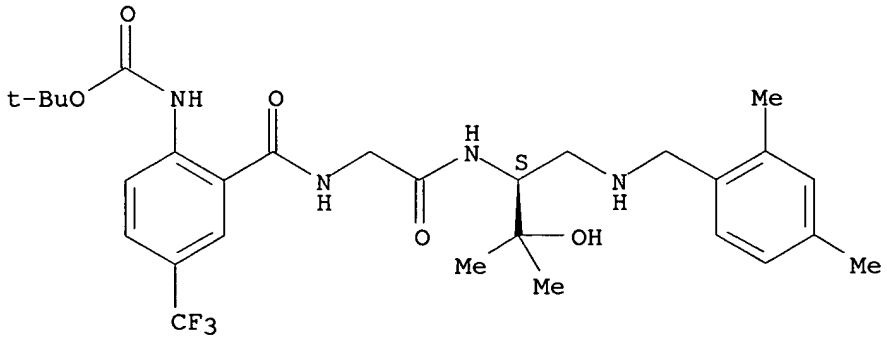
RN 439149-53-8 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-methoxypentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



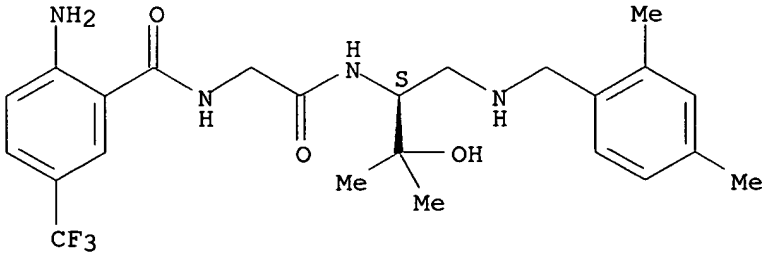
RN 439149-54-9 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-methylpropyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



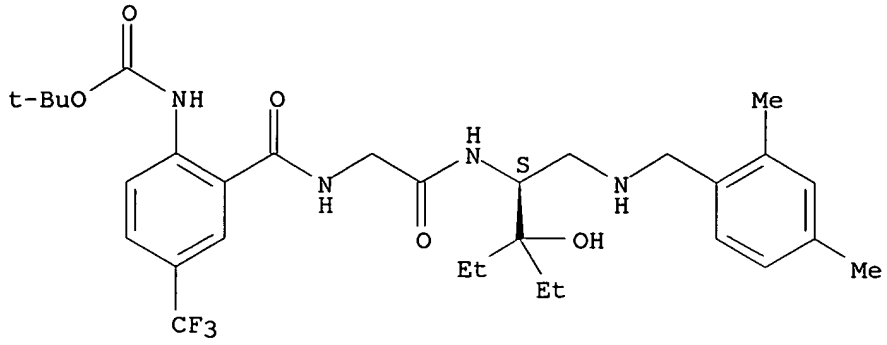
RN 439149-55-0 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-methylpropyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



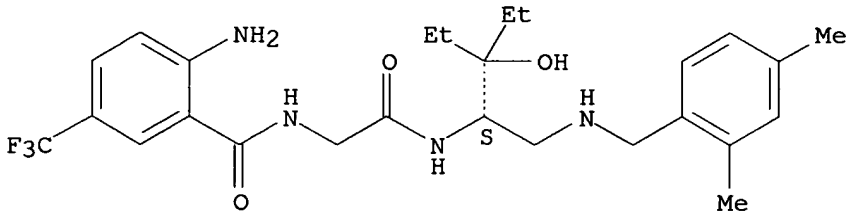
RN 439149-56-1 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-ethyl-2-hydroxybutyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



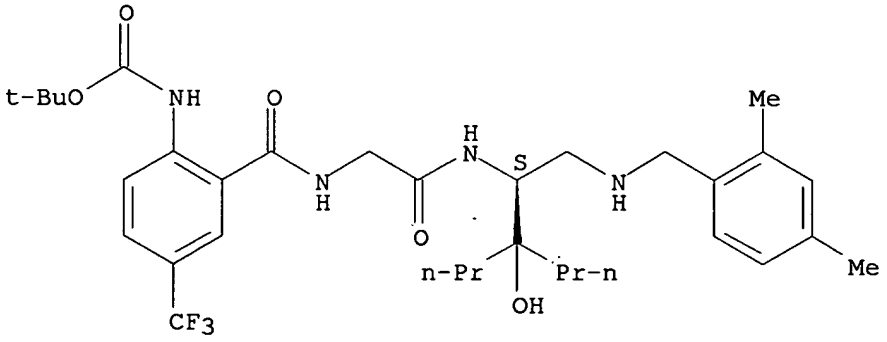
RN 439149-57-2 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-ethyl-2-hydroxybutyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



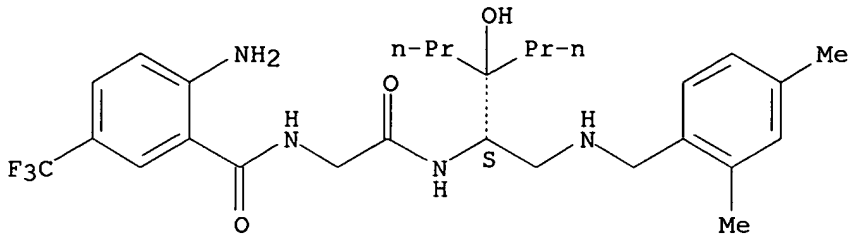
RN 439149-58-3 CAPLUS
CN Carbamic acid, [2-[[[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-propylpentyl]amino]-2-oxoethyl]amino]carbonyl]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



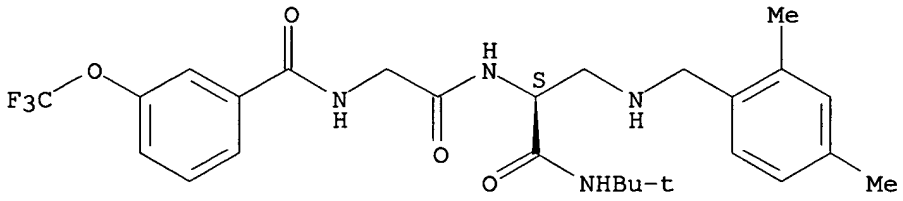
RN 439149-59-4 CAPLUS
CN Benzamide, 2-amino-N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-propylpentyl]amino]-2-oxoethyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



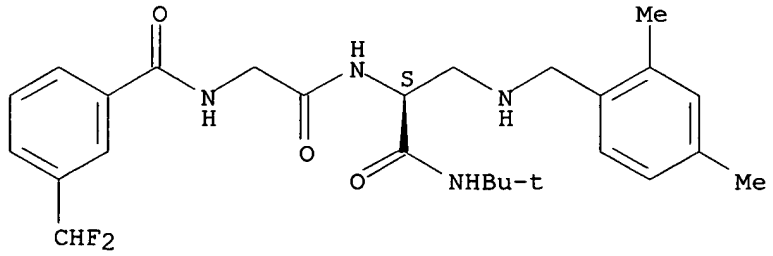
RN 439149-62-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethoxy)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



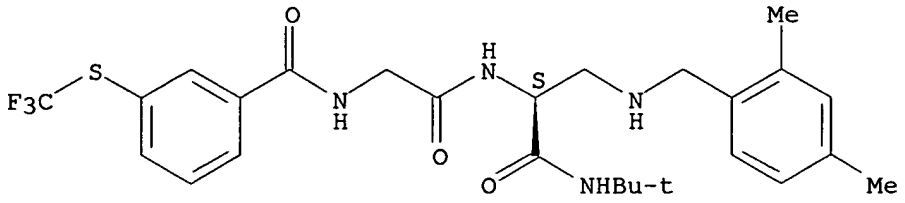
RN 439149-63-0 CAPLUS
CN L-Alaninamide, N-[3-(difluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



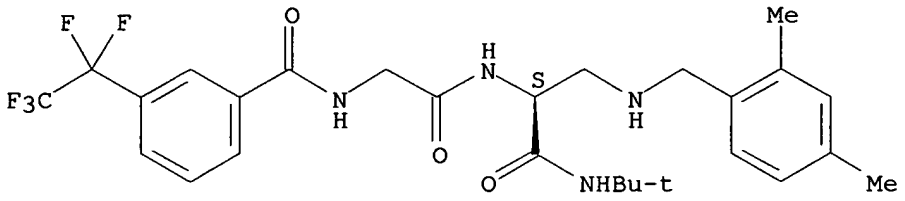
RN 439149-64-1 CAPLUS
CN L-Alaninamide, N-[3-[(trifluoromethyl)thio]benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



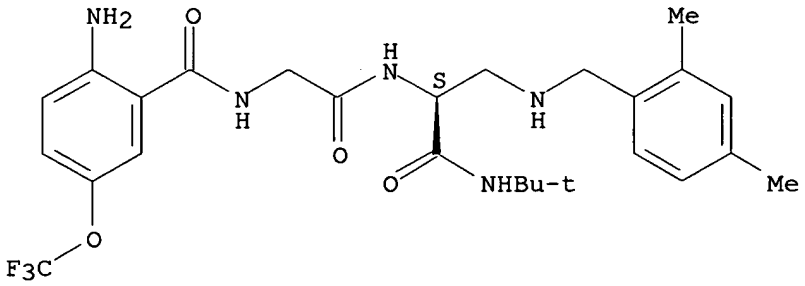
RN 439149-65-2 CAPLUS
CN L-Alaninamide, N-[3-(pentafluoroethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



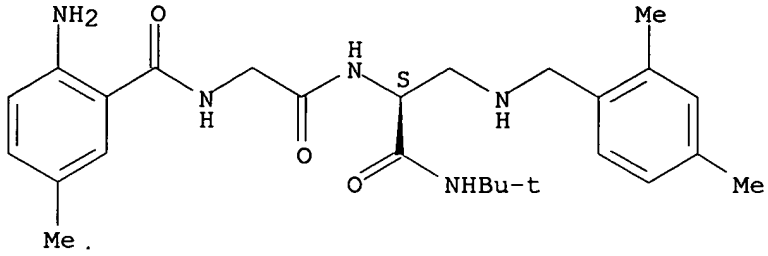
RN 439149-66-3 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethoxy)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



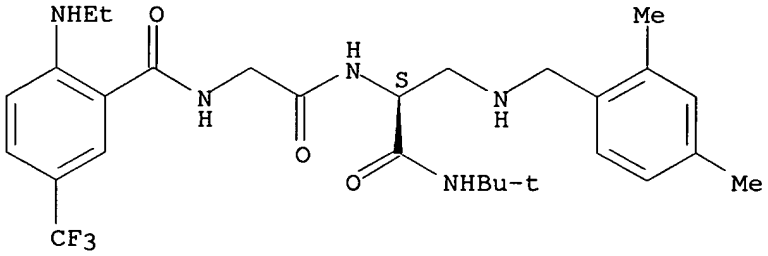
RN 439149-67-4 CAPLUS
CN L-Alaninamide, N-(2-amino-5-methylbenzoyl)glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



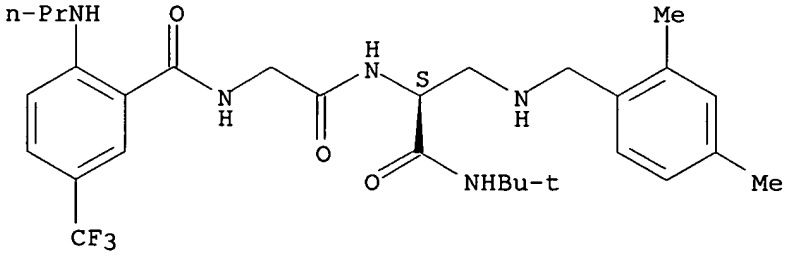
RN 439149-68-5 CAPLUS
CN L-Alaninamide, N-[2-(ethylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



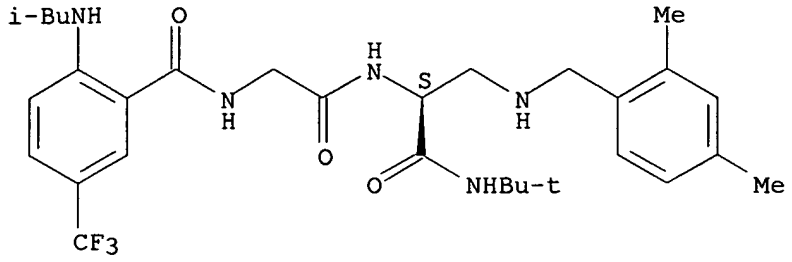
RN 439149-69-6 CAPLUS
CN L-Alaninamide, N-[2-(propylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



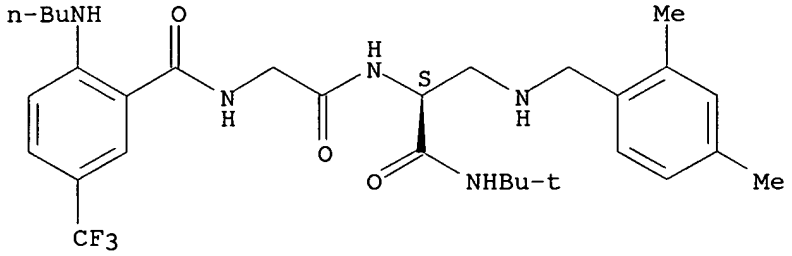
RN 439149-70-9 CAPLUS
CN L-Alaninamide, N-[2-[(2-methylpropyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



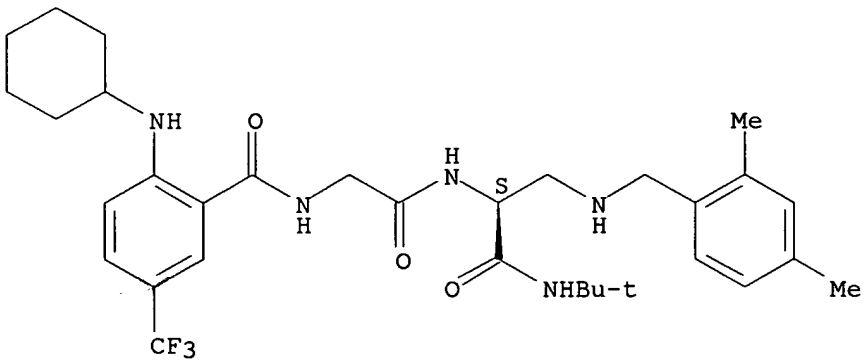
RN 439149-71-0 CAPLUS
CN L-Alaninamide, N-[2-(butylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



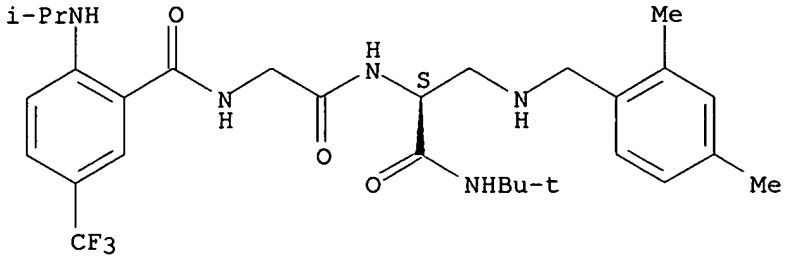
RN 439149-72-1 CAPLUS
CN L-Alaninamide, N-[2-(cyclohexylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



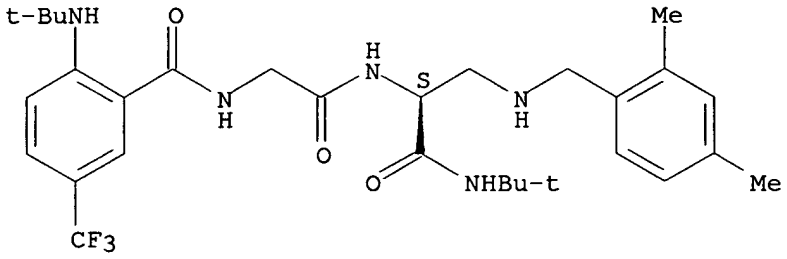
RN 439149-73-2 CAPLUS
CN L-Alaninamide, N-[2-[(1-methylethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



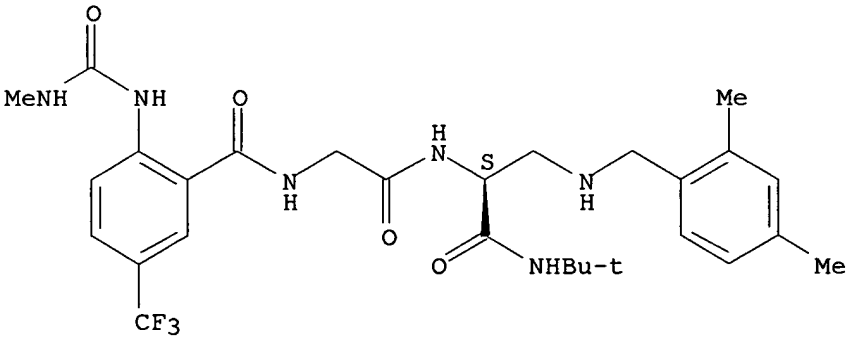
RN 439149-74-3 CAPLUS
CN L-Alaninamide, N-[2-[(1,1-dimethylethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



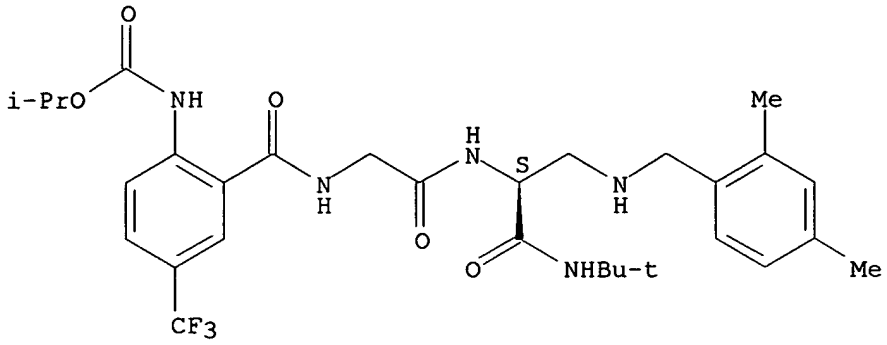
RN 439149-75-4 CAPLUS
CN L-Alaninamide, N-[2-[[(methylamino)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



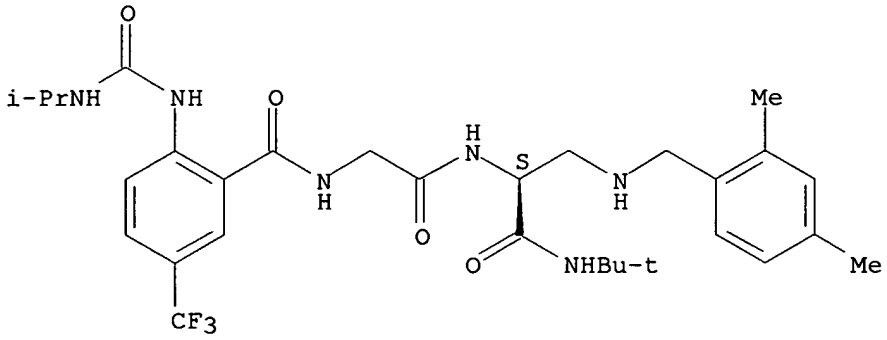
RN 439149-76-5 CAPLUS
CN L-Alaninamide, N-[2-[[(1-methylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



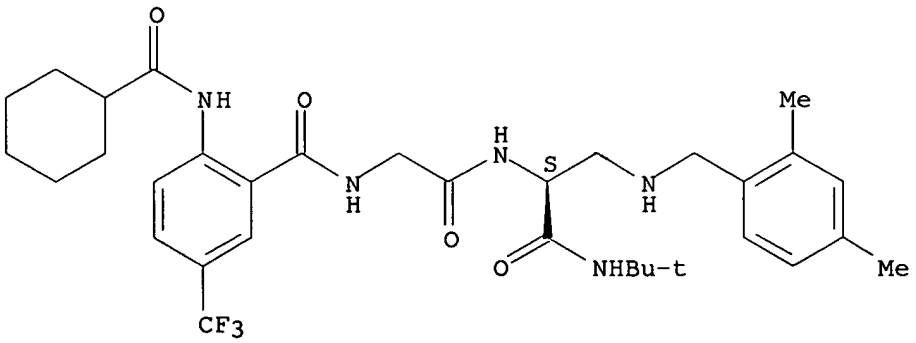
RN 439149-77-6 CAPLUS
CN L-Alaninamide, N-[2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439149-78-7 CAPLUS
CN L-Alaninamide, N-[2-[(cyclohexylcarbonyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

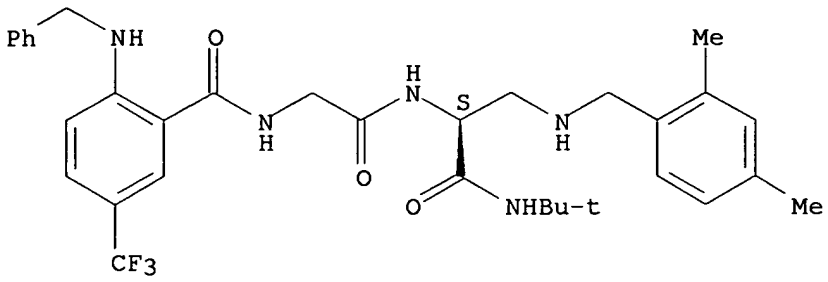
Absolute stereochemistry.



RN 439149-79-8 CAPLUS
CN L-Alaninamide, N-[2-[(phenylmethyl)amino]-5-(trifluoromethyl)benzoyl]glycy

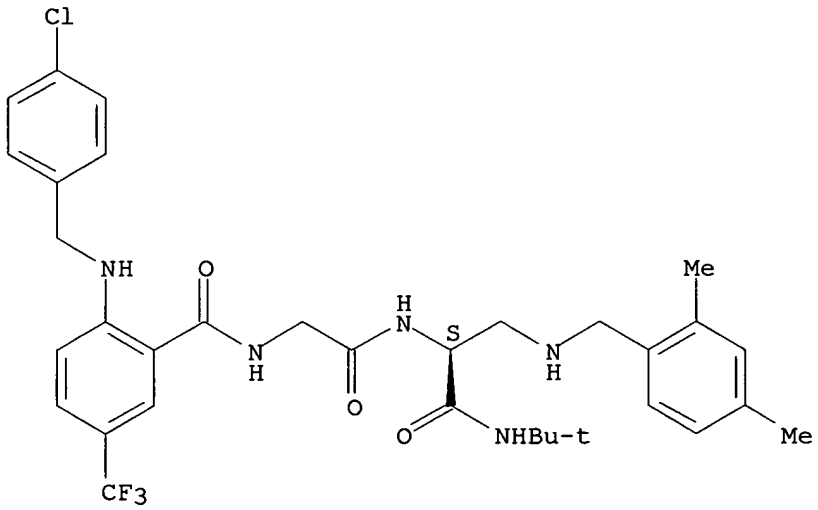
l-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



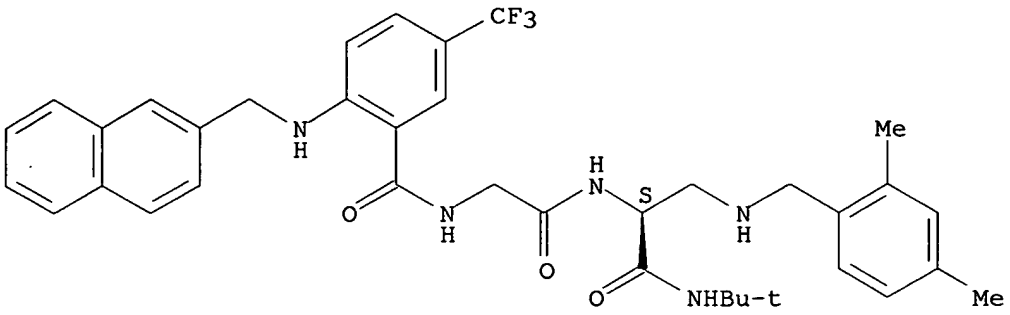
RN 439149-80-1 CAPLUS
CN L-Alaninamide, N-[2-[[(4-chlorophenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



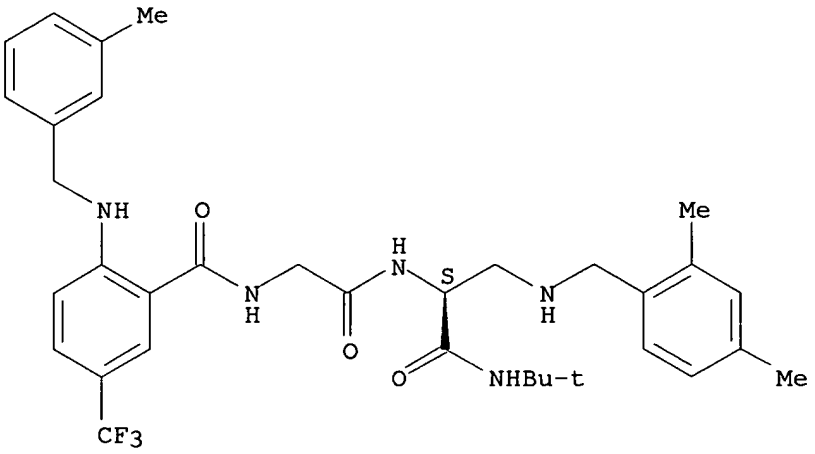
RN 439149-81-2 CAPLUS
CN L-Alaninamide, N-[2-[(2-naphthalenylmethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



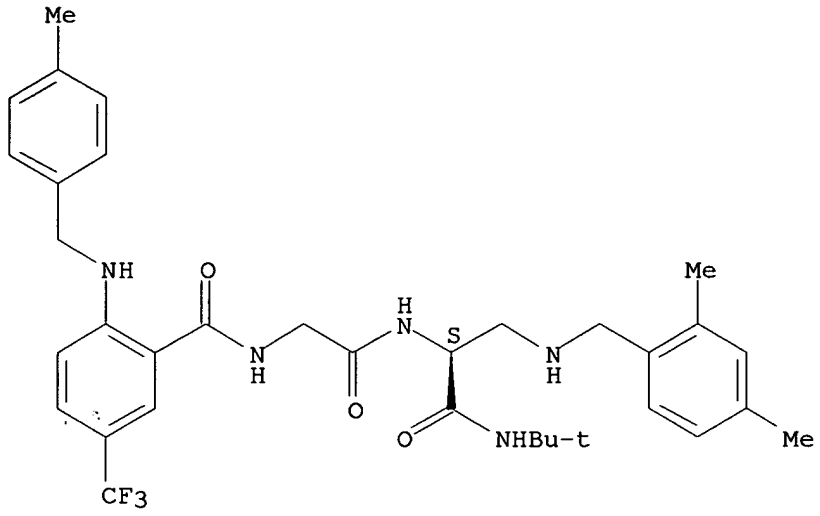
RN 439149-82-3 CAPLUS
CN L-Alaninamide, N-[2-[[(3-methylphenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



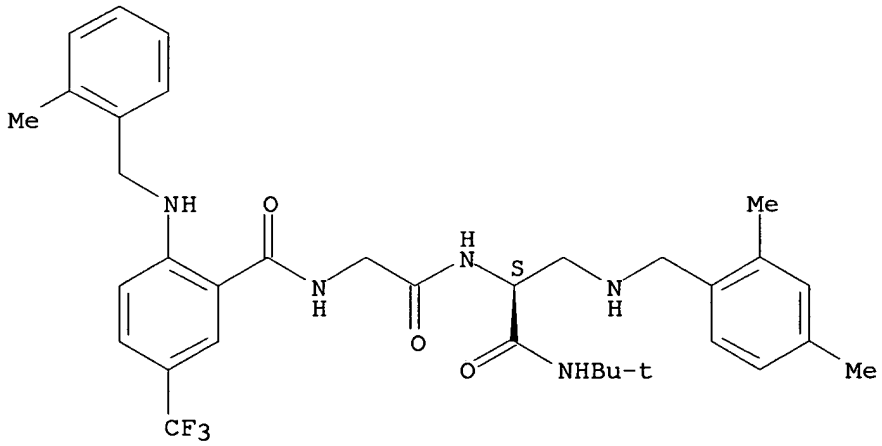
RN 439149-83-4 CAPLUS
CN L-Alaninamide, N-[2-[[(4-methylphenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



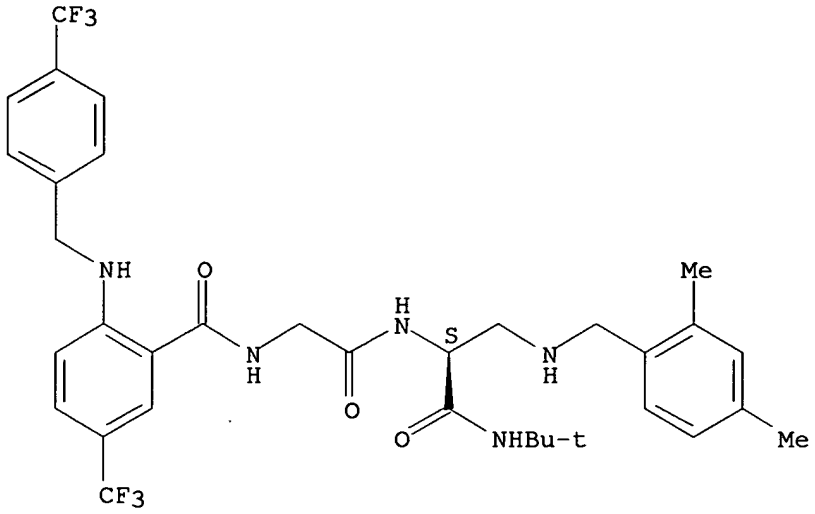
RN 439149-84-5 CAPLUS
CN L-Alaninamide, N-[2-[[(2-methylphenyl)methyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



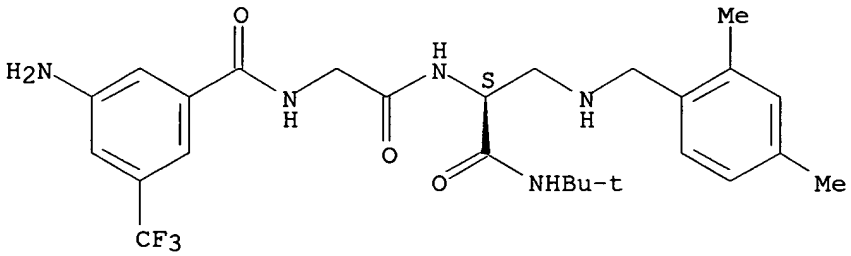
RN 439149-85-6 CAPLUS
CN L-Alaninamide, N-[5-(trifluoromethyl)-2-[[[4-(trifluoromethyl)phenyl]methyl]amino]benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



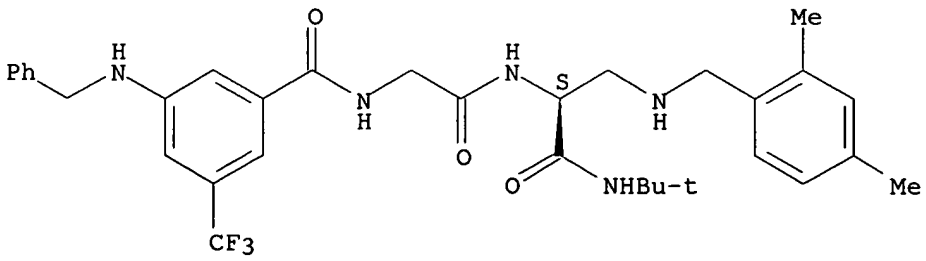
RN 439149-86-7 CAPLUS
CN L-Alaninamide, N-[3-amino-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439149-87-8 CAPLUS
CN L-Alaninamide, N-[3-[(phenylmethyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

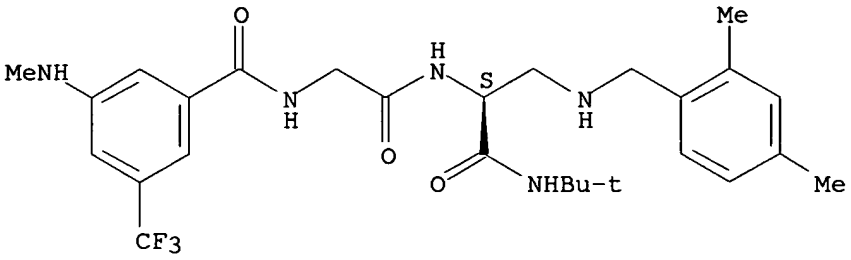
Absolute stereochemistry.



RN 439149-88-9 CAPLUS

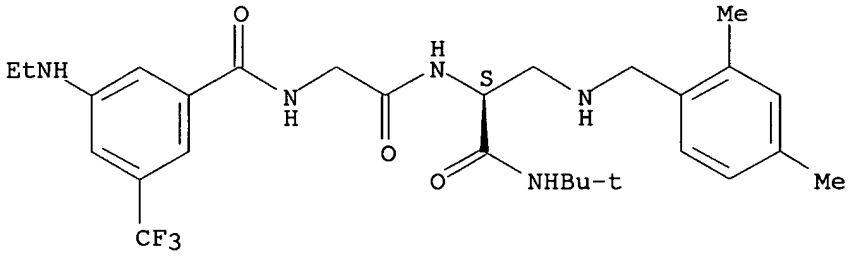
CN L-Alaninamide, N-[3-(methylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



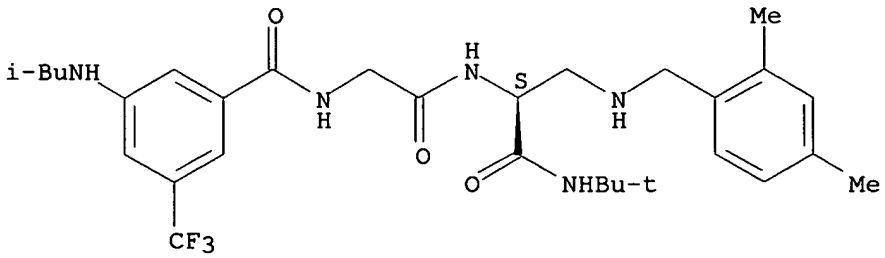
RN 439149-89-0 CAPLUS
CN L-Alaninamide, N-[3-(ethylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



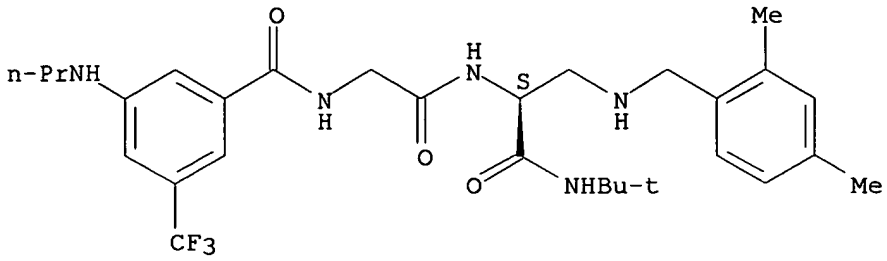
RN 439149-90-3 CAPLUS
CN L-Alaninamide, N-[3-[(2-methylpropyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



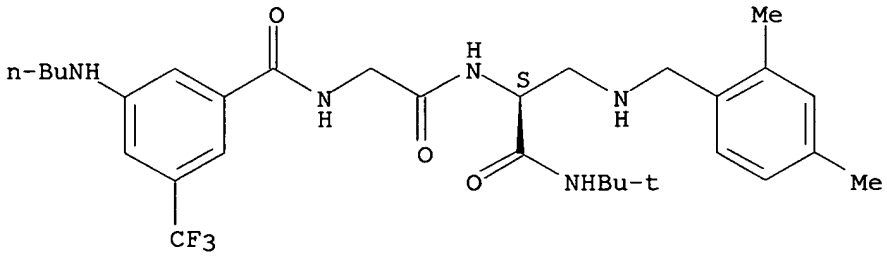
RN 439149-91-4 CAPLUS
CN L-Alaninamide, N-[3-(propylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



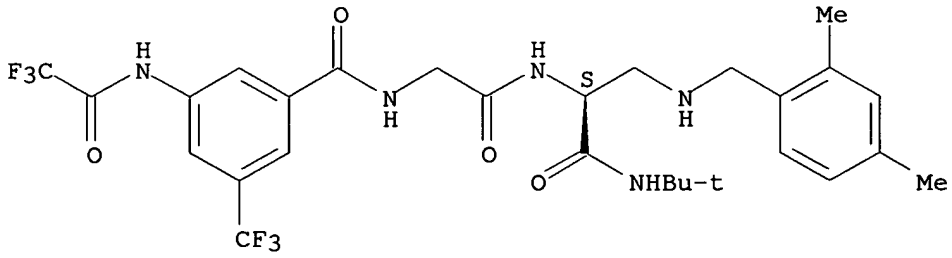
RN 439149-92-5 CAPLUS
CN L-Alaninamide, N-[3-(butylamino)-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



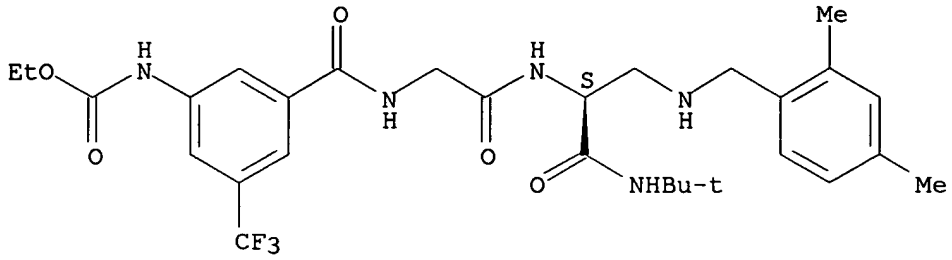
RN 439149-93-6 CAPLUS
CN L-Alaninamide, N-[3-[(trifluoroacetyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



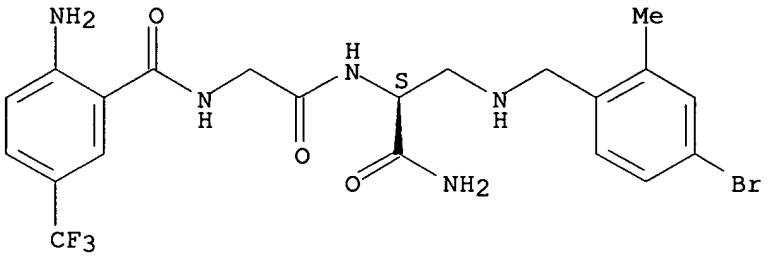
RN 439149-94-7 CAPLUS
CN L-Alaninamide, N-[3-[(ethoxycarbonyl)amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



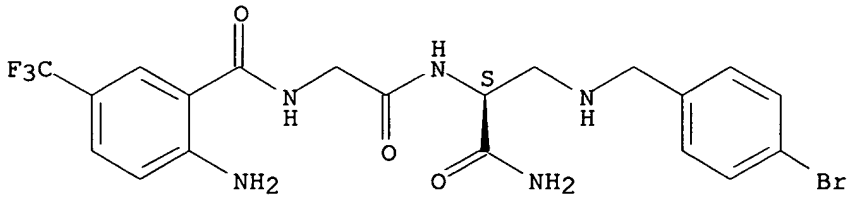
RN 439149-95-8 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



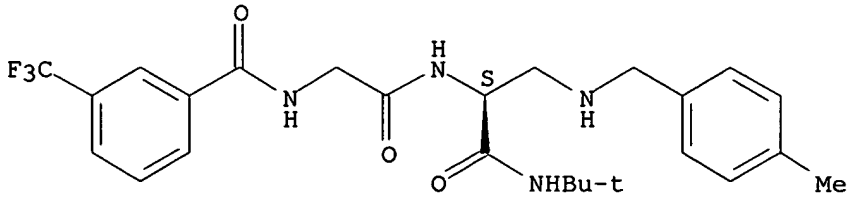
RN 439149-96-9 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromophenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



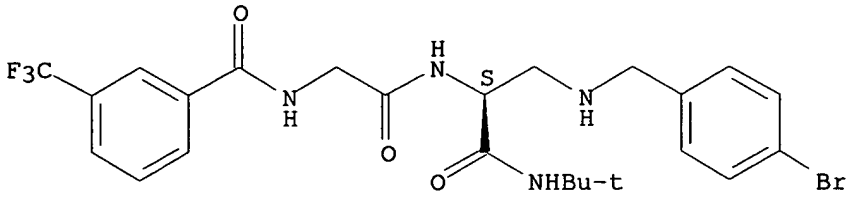
RN 439149-97-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



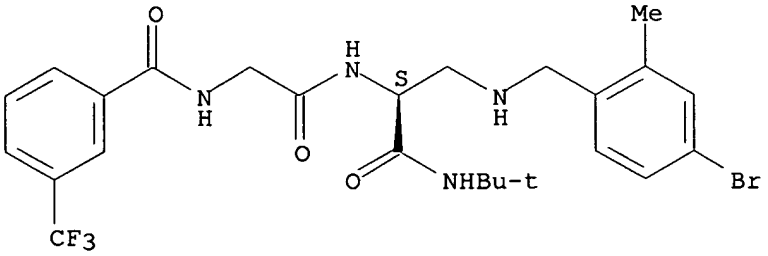
RN 439149-98-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromophenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



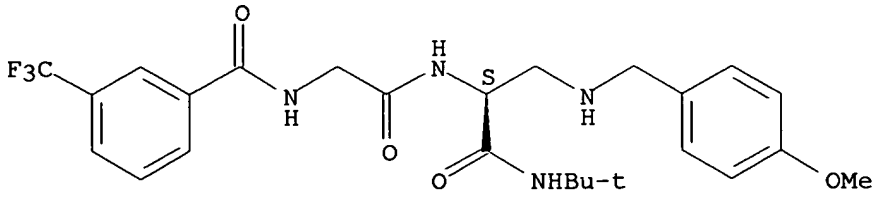
RN 439149-99-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-bromo-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



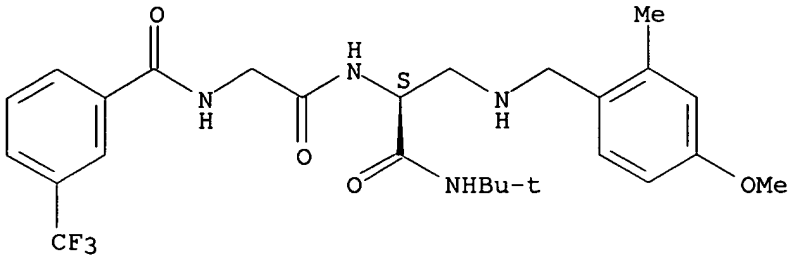
RN 439150-00-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methoxyphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



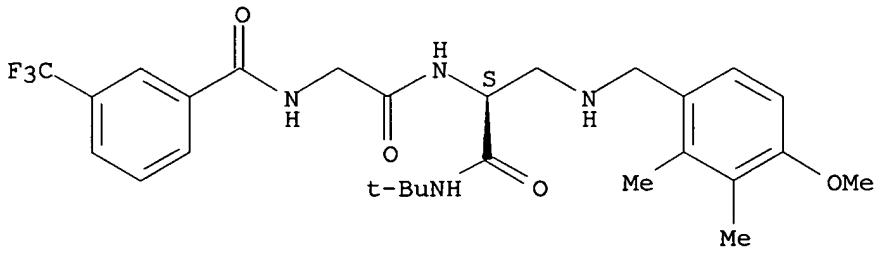
RN 439150-01-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methoxy-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



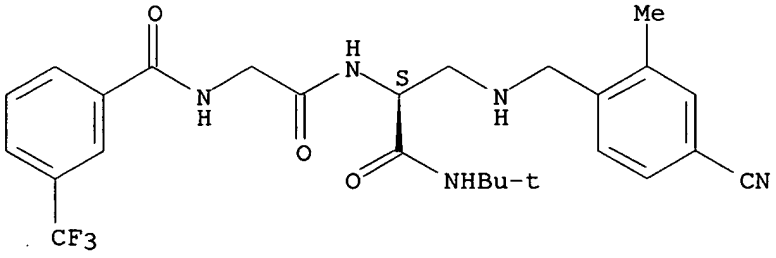
RN 439150-03-5 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-methoxy-2,3-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



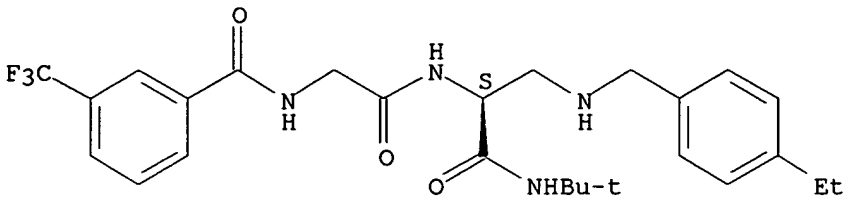
RN 439150-04-6 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-cyano-2-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



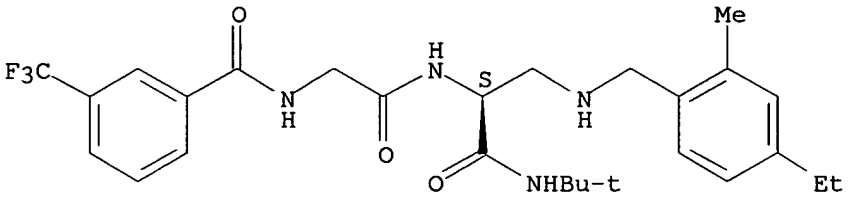
RN 439150-05-7 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-ethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



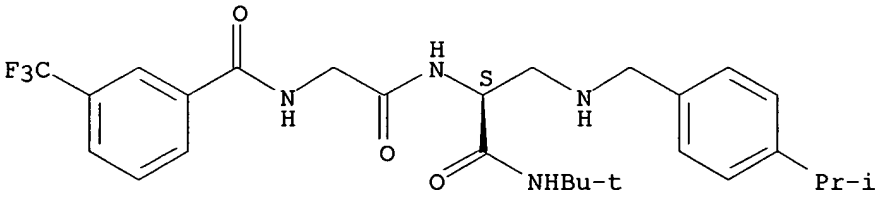
RN 439150-07-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(4-ethyl-2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



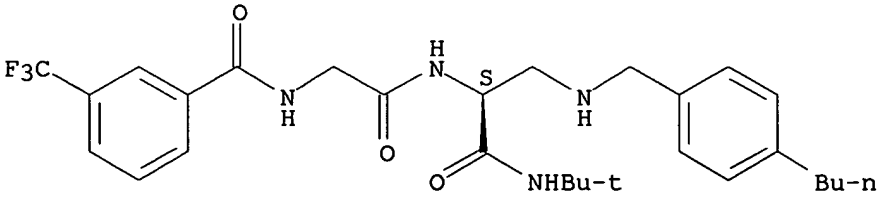
RN 439150-08-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(1-methylethyl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439150-09-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-butylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

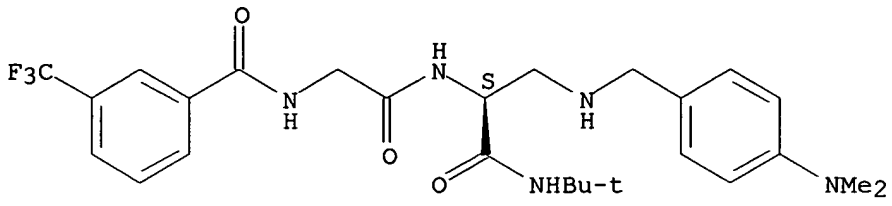
Absolute stereochemistry.



RN 439150-10-4 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[[4-(dimethylamino)phenyl]methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA

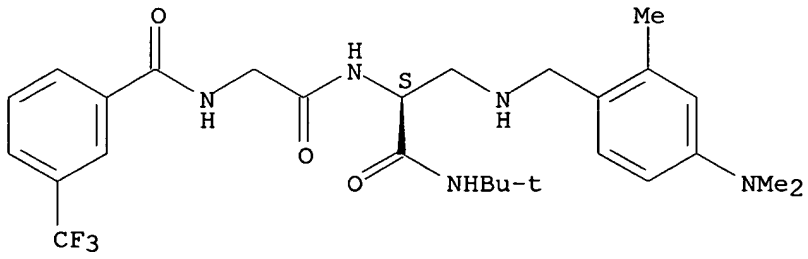
INDEX NAME)

Absolute stereochemistry.



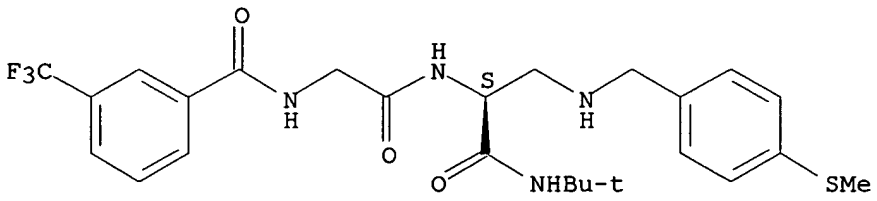
RN 439150-11-5 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[[4-(dimethylamino)-2-methylphenyl]methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



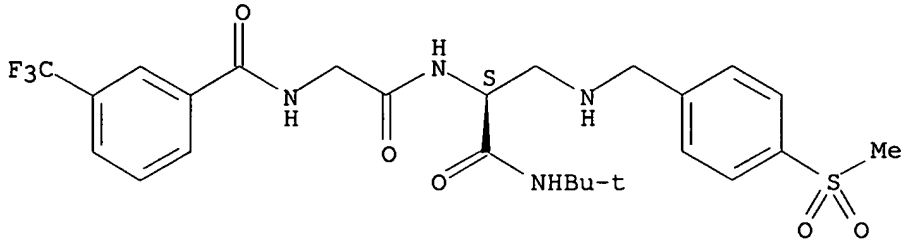
RN 439150-12-6 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(methylthio)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



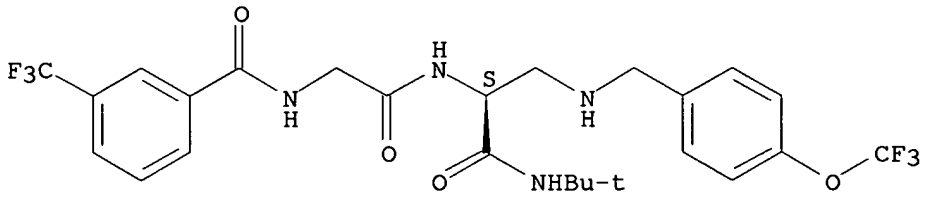
RN 439150-13-7 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(methylsulfonyl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



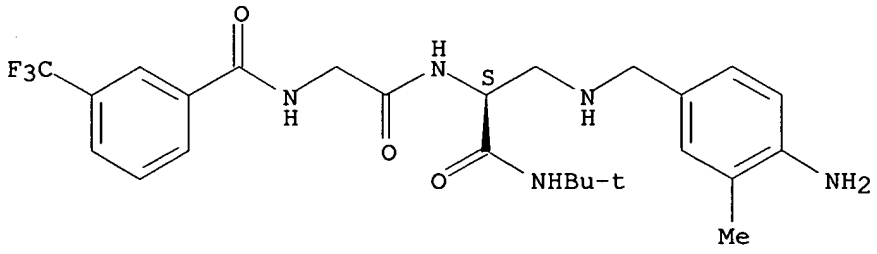
RN 439150-14-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[[4-(trifluoromethoxy)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



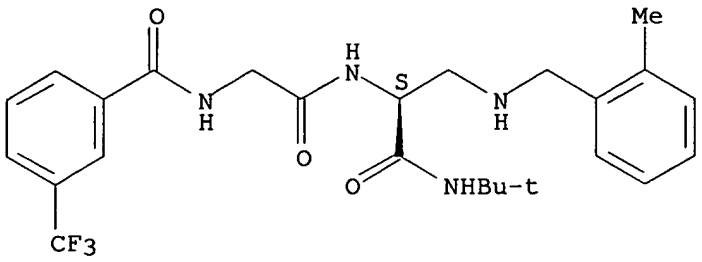
RN 439150-15-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-amino-3-methylphenyl)methyl]amino]-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



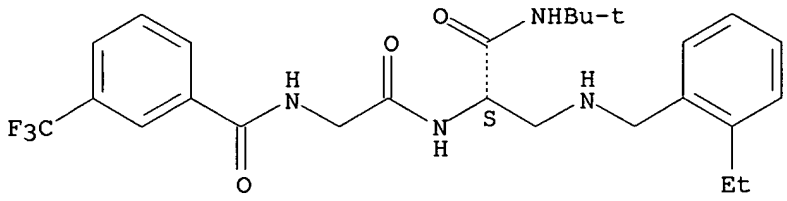
RN 439150-17-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2-methylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



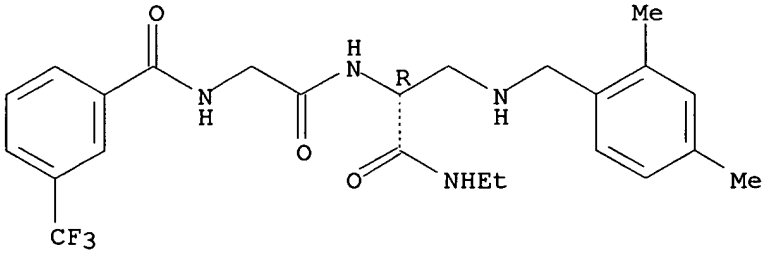
RN 439150-18-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2-ethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



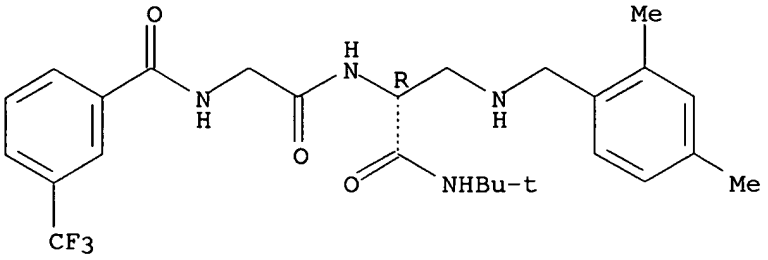
RN 439150-19-3 CAPLUS
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-ethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



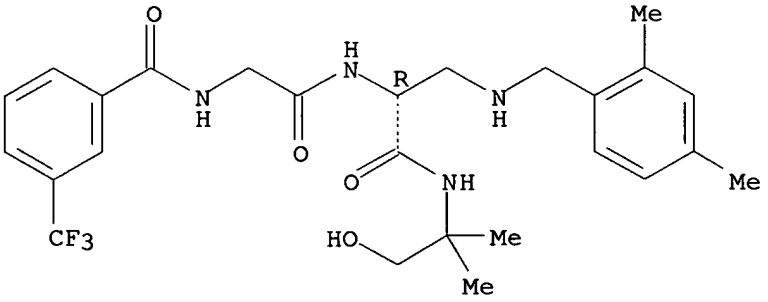
RN 439150-20-6 CAPLUS
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



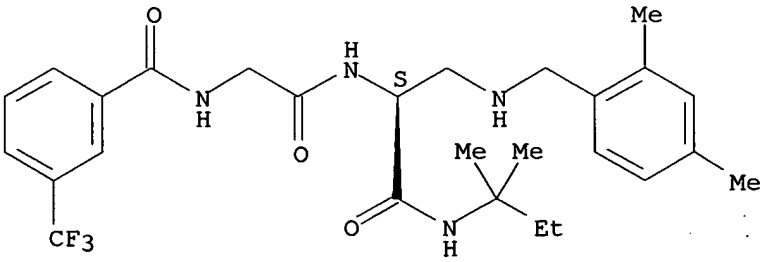
RN 439150-21-7 CAPLUS
CN D-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2-hydroxy-1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



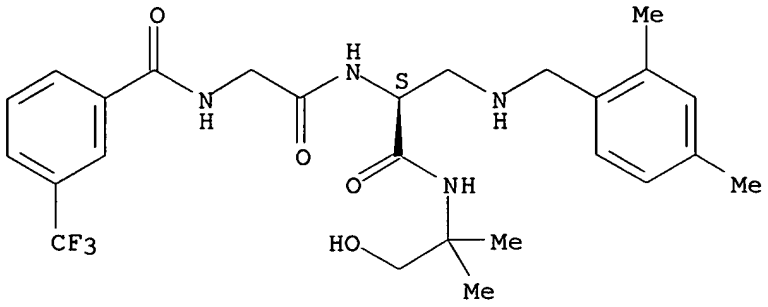
RN 439150-22-8 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1,1-dimethylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



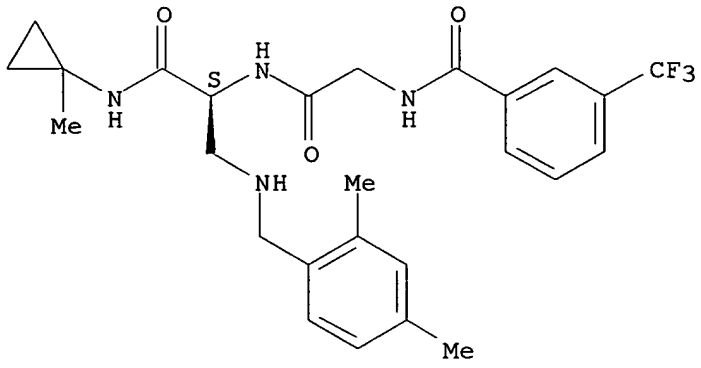
RN 439150-23-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2-hydroxy-1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



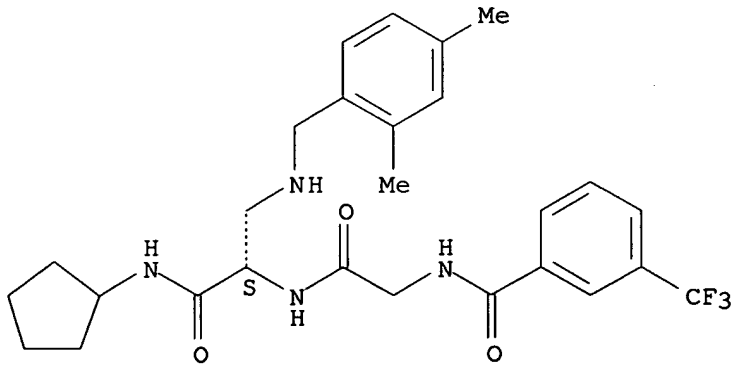
RN 439150-24-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1-methylcyclopropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439150-25-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclopentyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

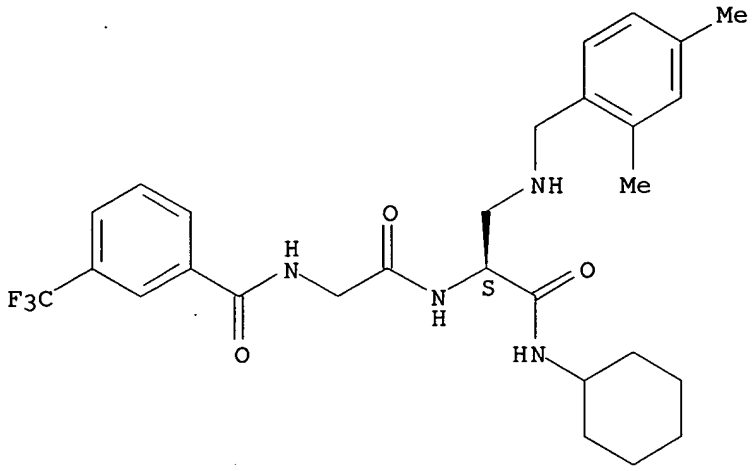
Absolute stereochemistry.



RN 439150-26-2 CAPLUS

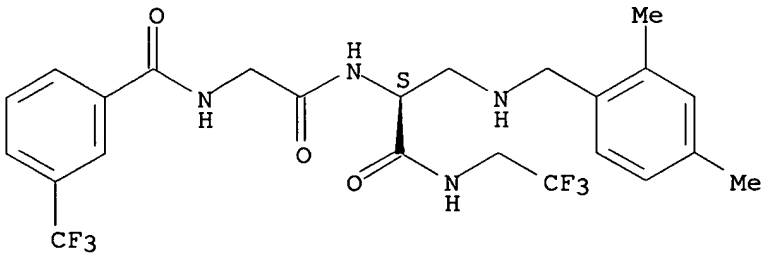
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-cyclohexyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



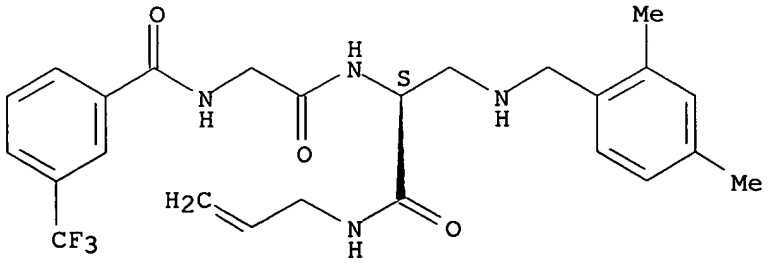
RN 439150-27-3 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



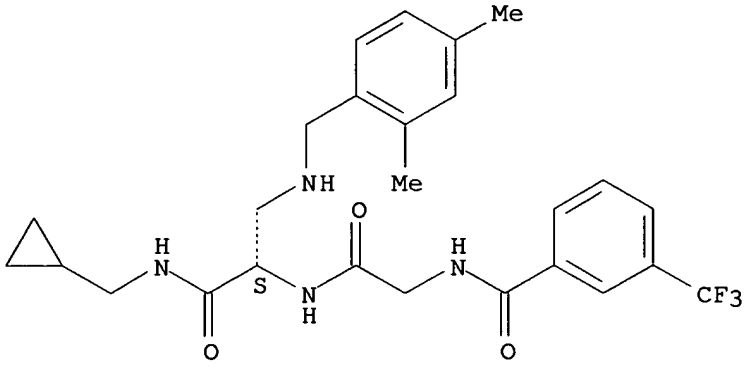
RN 439150-28-4 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-2-propenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



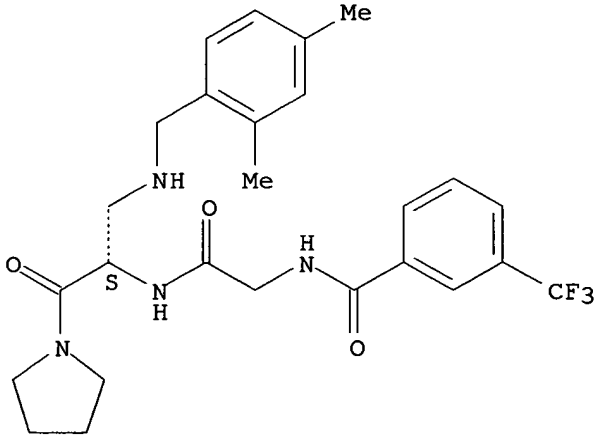
RN 439150-29-5 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(cyclopropylmethyl)-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



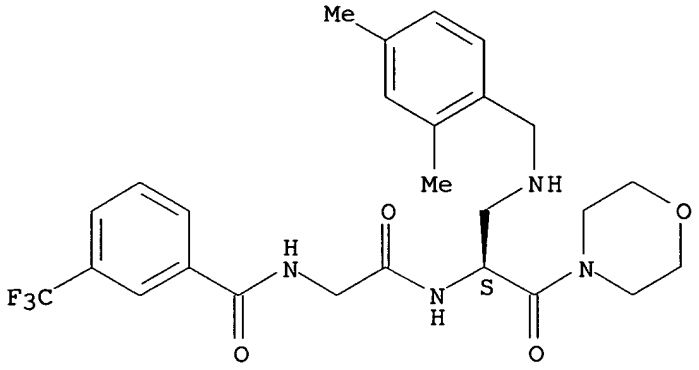
RN 439150-31-9 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-oxo-2-(1-pyrrolidinyl)ethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



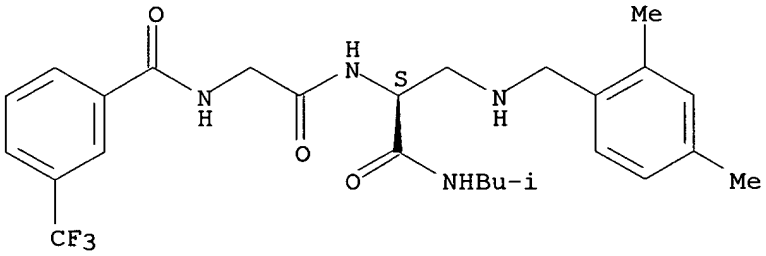
RN 439150-32-0 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-(4-morpholinyl)-2-oxoethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



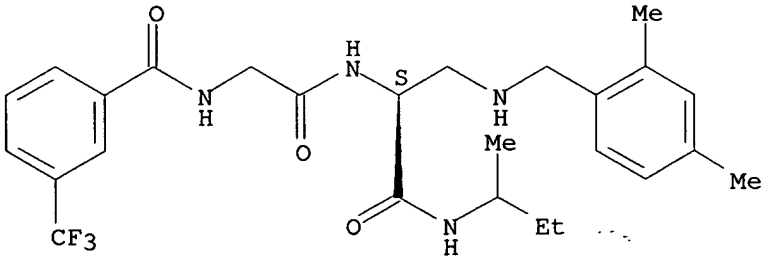
RN 439150-33-1 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



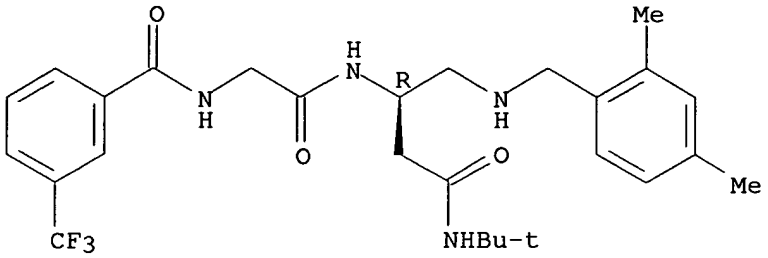
RN 439150-34-2 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-(1-methylpropyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



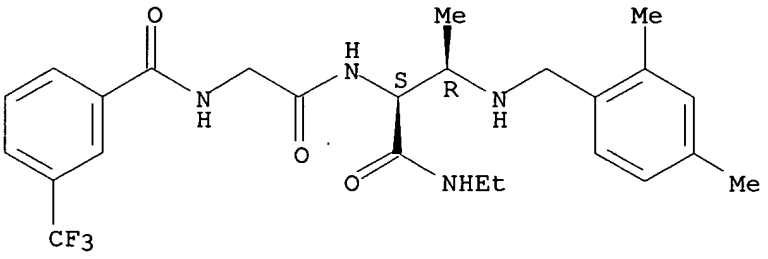
RN 439150-35-3 CAPLUS
CN Benzamide, N-[2-[[(1R)-3-[(1,1-dimethylethyl)amino]-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-3-oxopropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



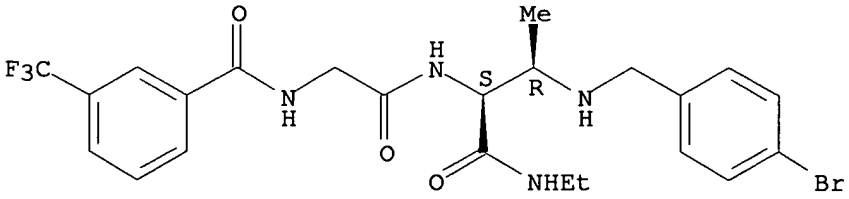
RN 439150-36-4 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-2-[[(2,4-dimethylphenyl)methyl]amino]-1-[(ethylamino)carbonyl]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



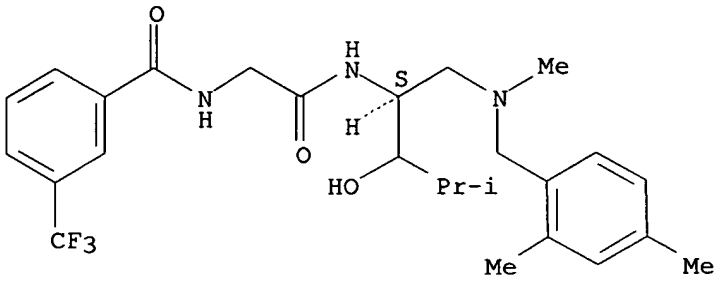
RN 439150-37-5 CAPLUS
CN Benzamide, N-[2-[[(1S,2R)-2-[[(4-bromophenyl)methyl]amino]-1-[(ethylamino)carbonyl]propyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



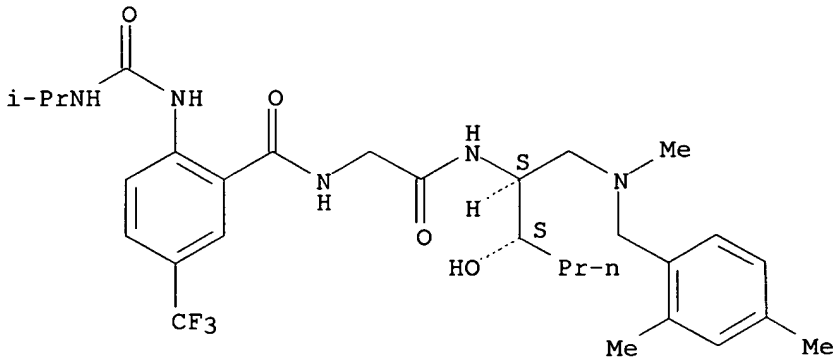
RN 439150-53-5 CAPLUS
CN D-glycero-Pentitol, 1,2,4,5-tetradeoxy-1-[{(2,4-dimethylphenyl)methyl]methylamino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]-, (3.xi.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



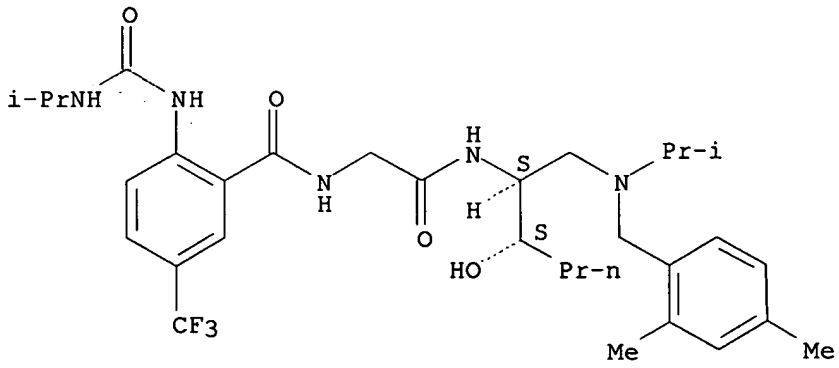
RN 439150-54-6 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl]methylamino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



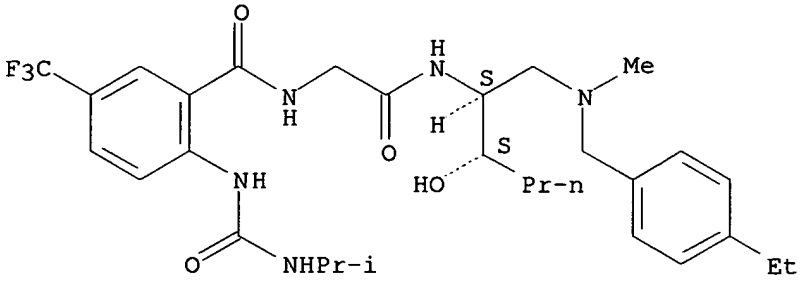
RN 439150-55-7 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(2,4-dimethylphenyl)methyl](1-methylethyl)amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



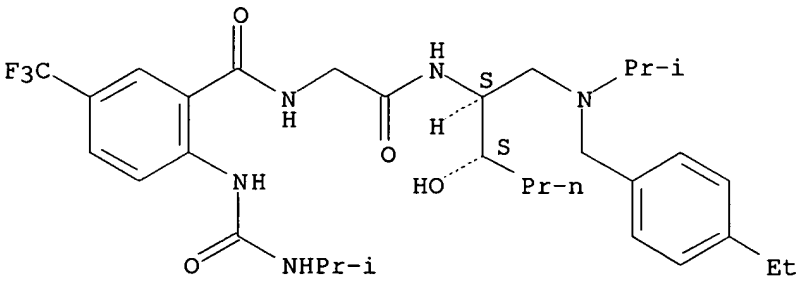
RN 439150-56-8 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl]methylamino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



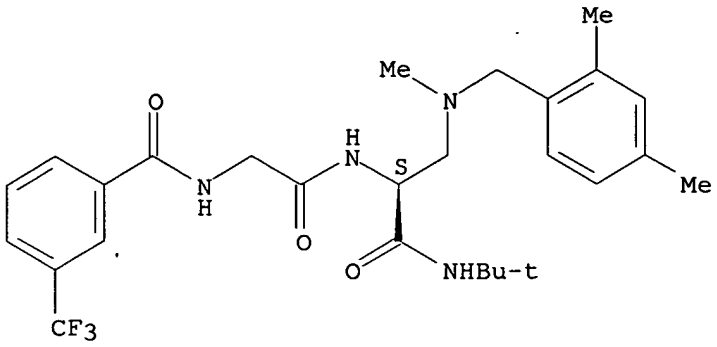
RN 439150-57-9 CAPLUS
CN Benzamide, N-[2-[[(1S,2S)-1-[[[(4-ethylphenyl)methyl](1-methylethyl)amino]methyl]-2-hydroxypentyl]amino]-2-oxoethyl]-2-[[[(1-methylethyl)amino]carbonyl]amino]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

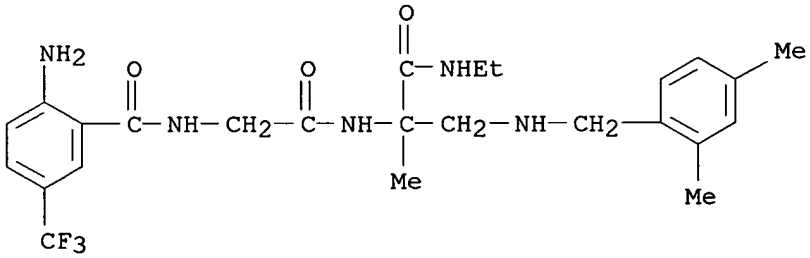


RN 439150-58-0 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl]methylamino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

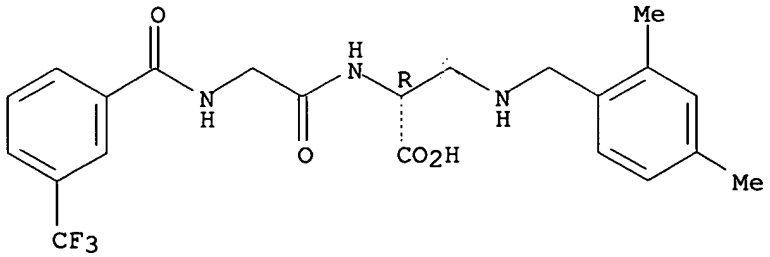


RN 439150-65-9 CAPLUS
CN Alaninamide, N-[2-amino-5-(trifluoromethyl)benzoyl]glycyl-2-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-N-ethyl- (9CI) (CA INDEX NAME)



IT **439150-68-2P 439150-69-3P 439150-86-4P**
439150-88-6P 439150-90-0P 439150-92-2P
439151-00-5P 439151-01-6P 439151-31-2P
439151-39-0P 439151-84-5P 439152-00-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of amino acid-related diamines as modulators of chemokine receptor activity)
RN 439150-68-2 CAPLUS
CN D-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]- (9CI) (CA INDEX NAME)

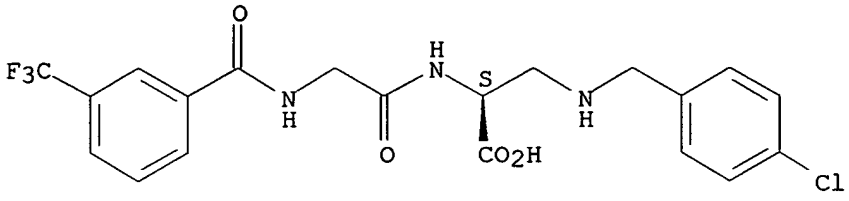
Absolute stereochemistry.



RN 439150-69-3 CAPLUS
CN L-Alanine, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(4-

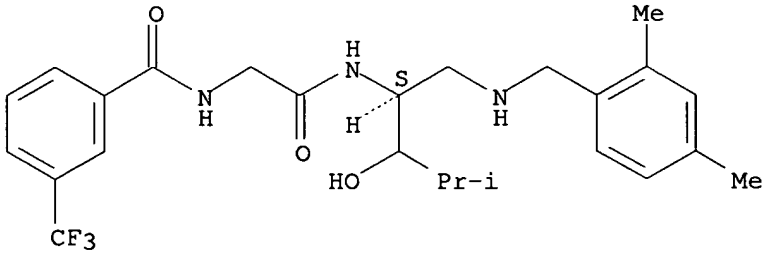
chlorophenyl)methyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



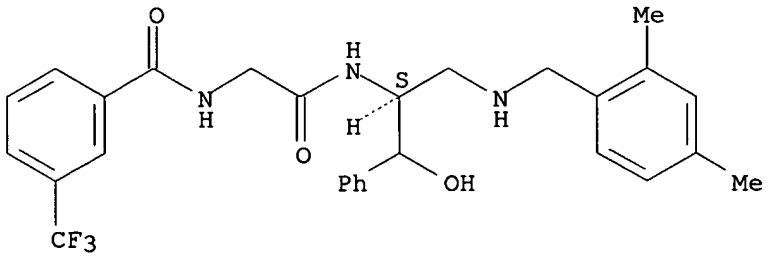
RN 439150-86-4 CAPLUS
CN D-glycero-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl]amino]-4-methyl-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]-, (3.xi.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



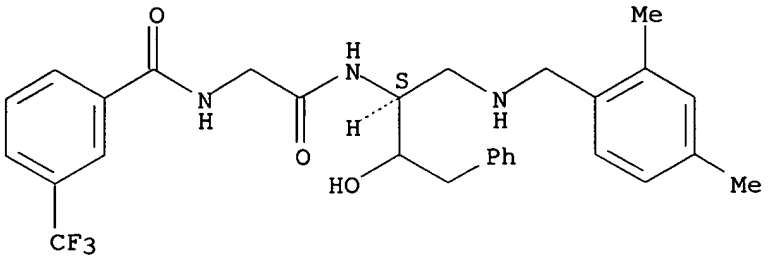
RN 439150-88-6 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-2-phenylethyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



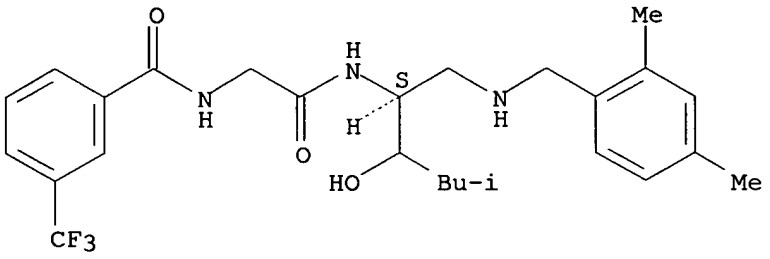
RN 439150-90-0 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-3-phenylpropyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



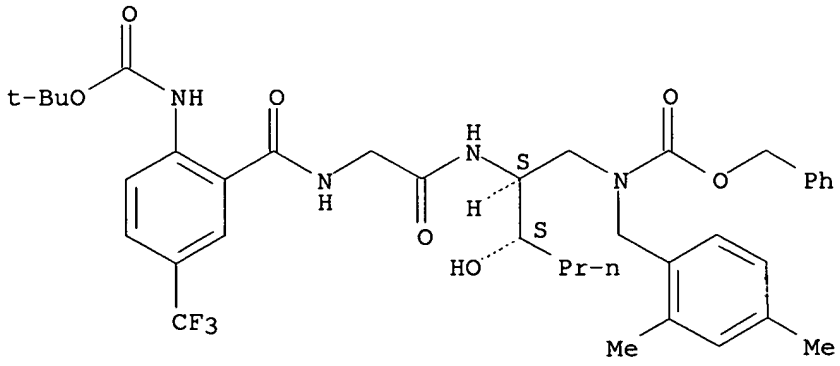
RN 439150-92-2 CAPLUS
CN Benzamide, N-[2-[[(1S)-1-[[[(2,4-dimethylphenyl)methyl]amino]methyl]-2-hydroxy-4-methylpentyl]amino]-2-oxoethyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



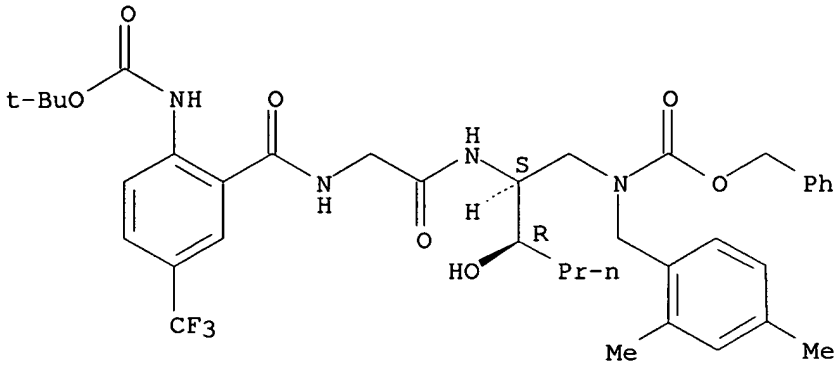
RN 439151-00-5 CAPLUS
CN Carbamic acid, [(2S,3S)-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-3-hydroxyhexyl][(2,4-dimethylphenyl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



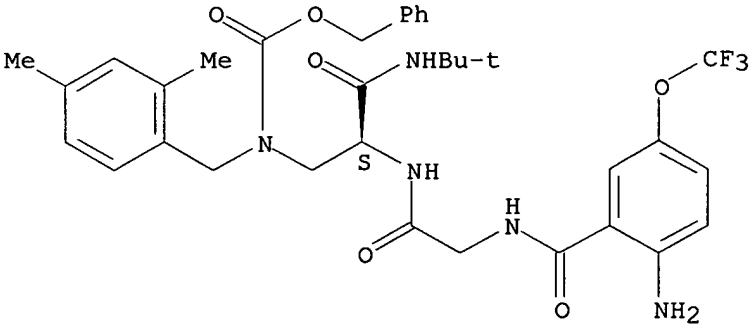
RN 439151-01-6 CAPLUS
CN Carbamic acid, [(2S,3R)-2-[[[[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]amino]acetyl]amino]-3-hydroxyhexyl][(2,4-dimethylphenyl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



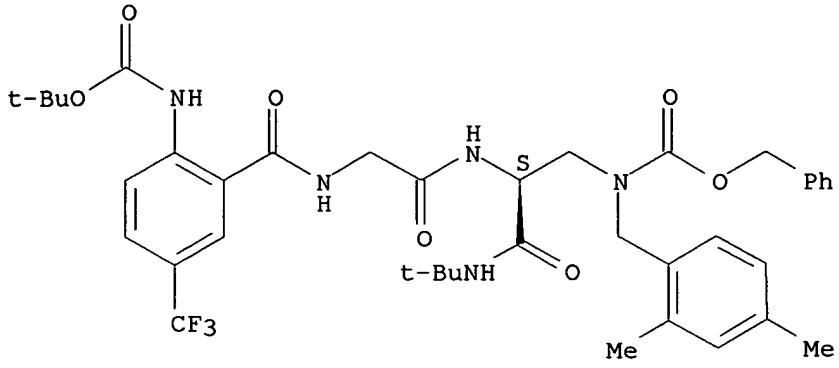
RN 439151-31-2 CAPLUS
CN L-Alaninamide, N-[2-amino-5-(trifluoromethoxy)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl][(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



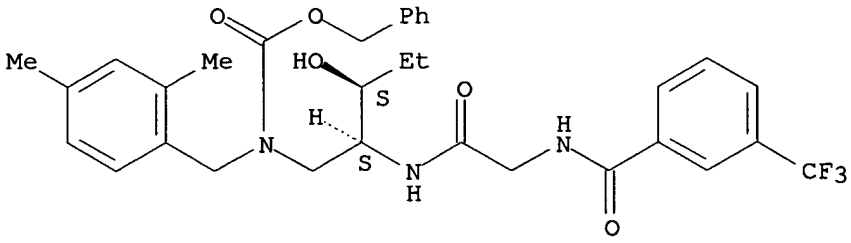
RN 439151-39-0 CAPLUS
CN L-Alaninamide, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]-5-(trifluoromethyl)benzoyl]glycyl-N-(1,1-dimethylethyl)-3-[[(2,4-dimethylphenyl)methyl][(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



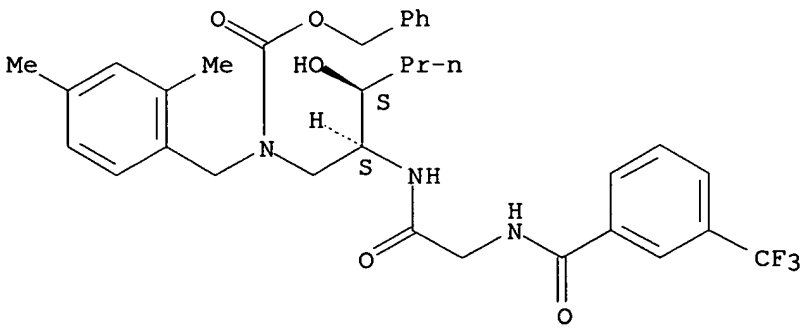
RN 439151-84-5 CAPLUS
CN L-threo-Pentitol, 1,2,4,5-tetradeoxy-1-[[(2,4-dimethylphenyl)methyl][(phenylmethoxy)carbonyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



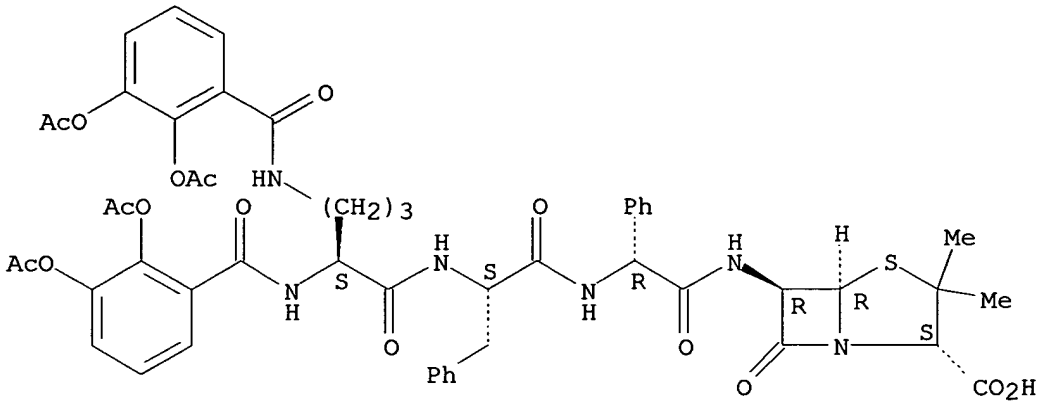
RN 439152-00-8 CAPLUS
CN Carbamic acid, [(2,4-dimethylphenyl)methyl][(2S,3S)-3-hydroxy-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]hexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



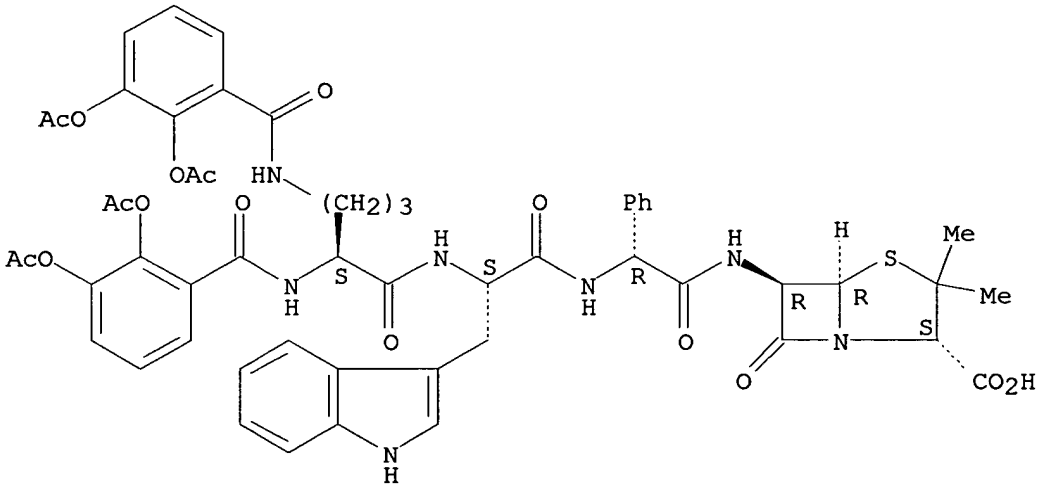
L27 ANSWER 5 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2002:251248 CAPLUS
DN 137:60114
TI New synthetic siderophores and their .beta.-lactam conjugates based on diamino acids and dipeptides
AU Wittmann, S.; Schnabelrauch, M.; Scherlitz-Hofmann, I.; Mollmann, U.; Ankel-Fuchs, D.; Heinisch, L.
CS Hans Knoll Institute for Natural Product Research, Jena, Jena, D-07745, Germany
SO Bioorganic & Medicinal Chemistry (2002), 10(6), 1659-1670
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 137:60114
AB Linking of siderophores to antibiotics improves the penetration and therefore increases the antibacterial activity of the antibiotics. We synthesized the acylated catecholates and hydroxamates as siderophore components for antibiotic conjugates to reduce side effects of unprotected catecholate and hydroxamate moieties. In this paper, we report on bis- and tris-catecholates and mixed catecholate hydroxamates based on diamino acids or dipeptides. These compds. were active as siderophores in a growth promotion assay under Fe limitation. Most of the conjugates with .beta.-lactams showed high in vitro activity against Gram-neg. bacteria, esp. Pseudomonas aeruginosa, Escherichia coli, Klebsiella pneumoniae, Serratia marcescens, and Stenotrophomonas maltophilia. The compds. with enhanced antibacterial activity use active Fe uptake routes to penetrate the bacterial outer membrane barrier, demonstrated by assays with mutants deficient in components of the Fe transport system. Correlation between chem. structure and biol. activity was studied.
IT **439152-40-6P 439152-41-7P 439152-43-9P**
439152-44-0P 439152-48-4P 439152-49-5P
439152-50-8P 439152-51-9P
RL: BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(new synthetic siderophores and their .beta.-lactam conjugates based on diamino acids and dipeptides)
RN 439152-40-6 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-phenylalanyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



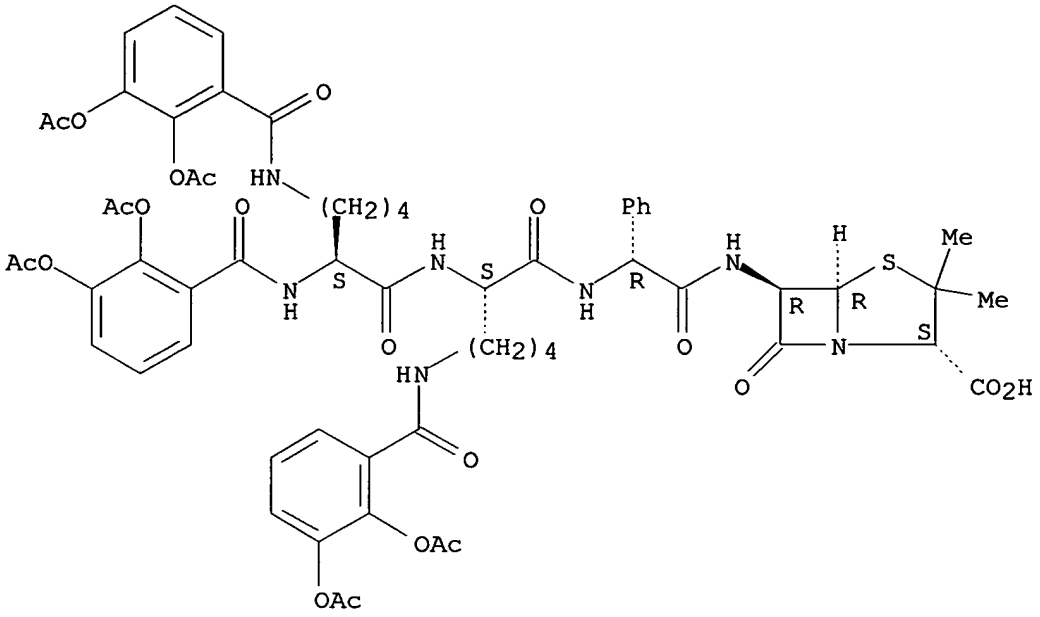
RN 439152-41-7 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-L-ornithyl-L-tryptophyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



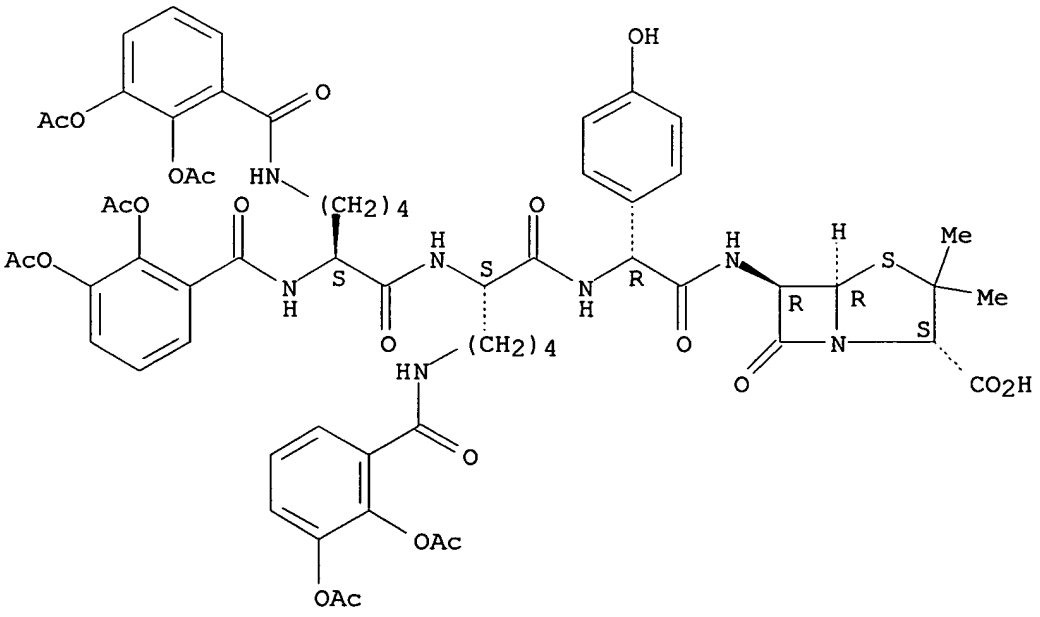
RN 439152-43-9 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N6-[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439152-44-0 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N6-[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-(4-hydroxyphenyl)-, (2R)- (9CI) (CA INDEX NAME)

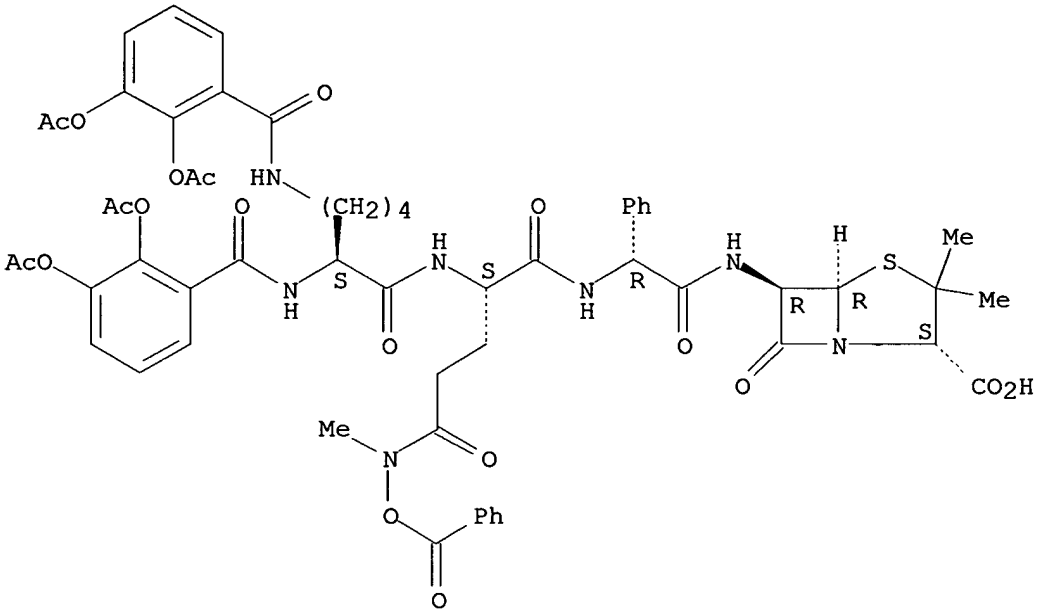
Absolute stereochemistry.



RN 439152-48-4 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-(benzoyloxy)-N-methyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-

azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

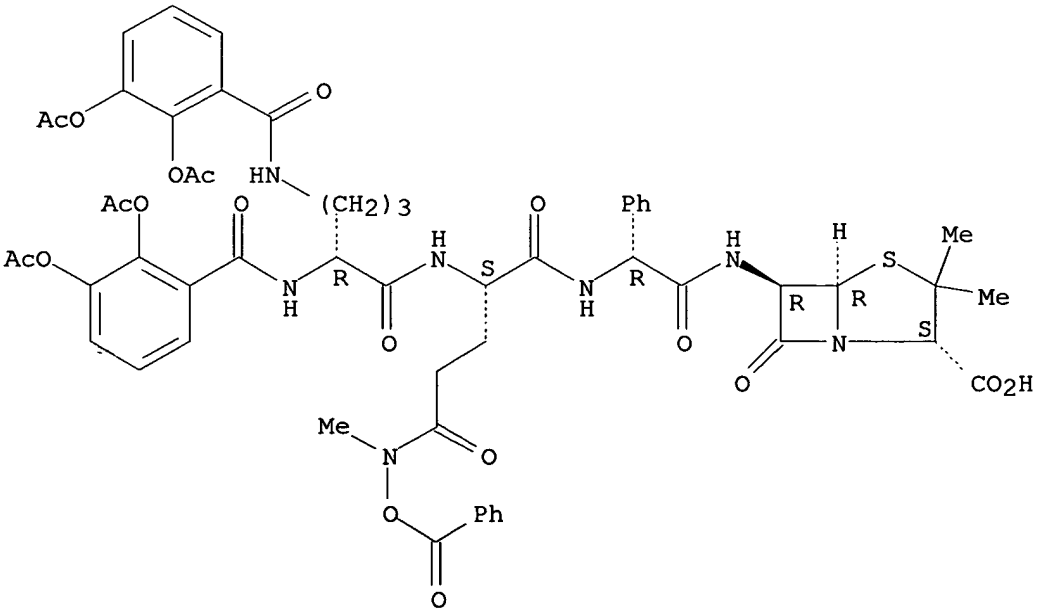
Absolute stereochemistry.



RN 439152-49-5 CAPLUS

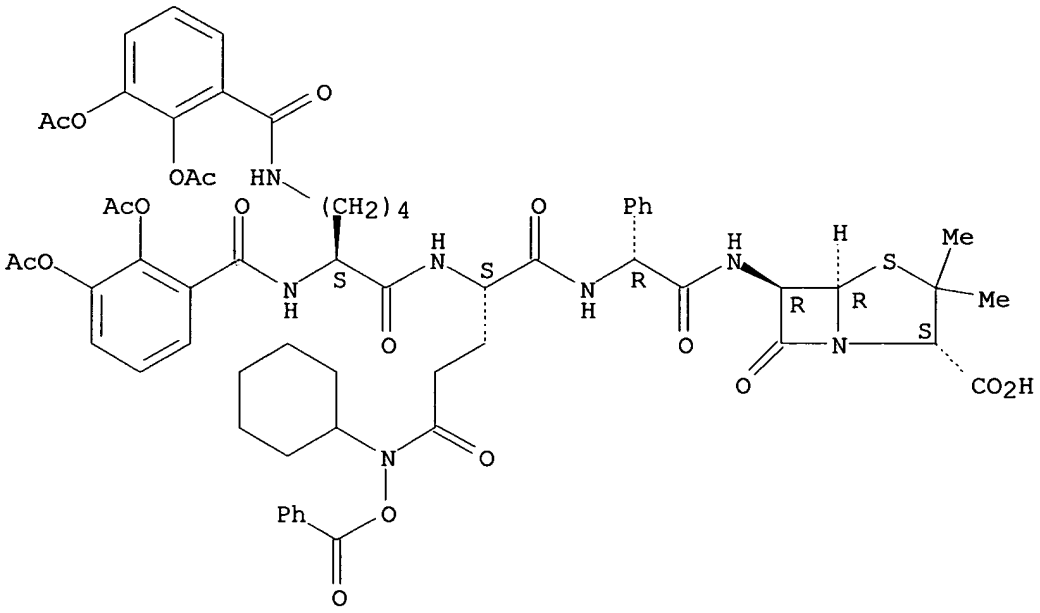
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-D-ornithyl-N-(benzoyloxy)-N-methyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



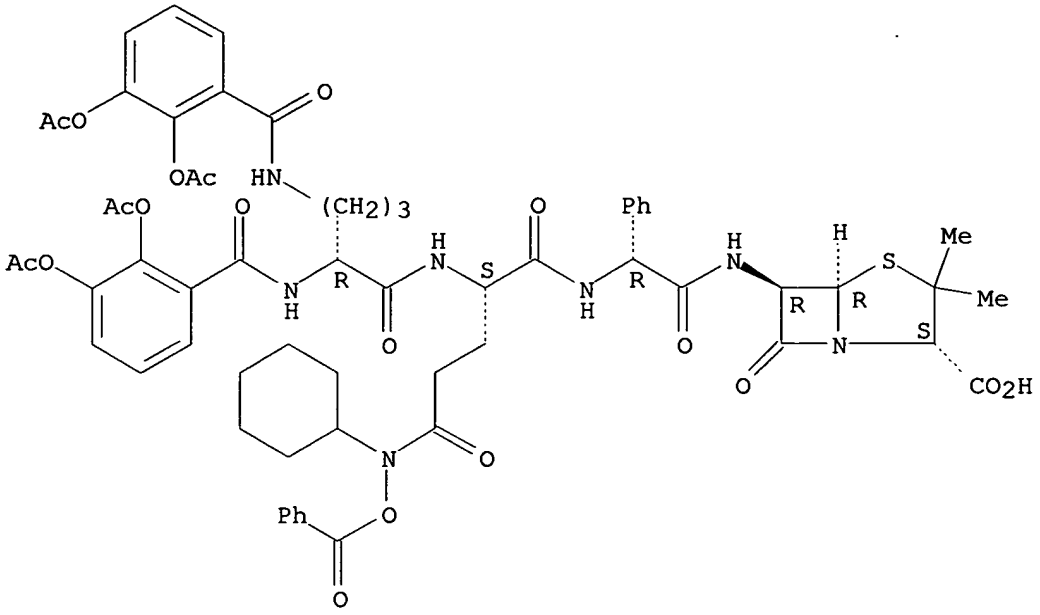
RN 439152-50-8 CAPLUS
CN Glycinamide, N2,N6-bis[2,3-bis(acetyloxy)benzoyl]-L-lysyl-N-(benzoyloxy)-N-cyclohexyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 439152-51-9 CAPLUS
CN Glycinamide, N2,N5-bis[2,3-bis(acetyloxy)benzoyl]-D-ornithyl-N-(benzoyloxy)-N-cyclohexyl-L-glutaminyl-N-[(2S,5R,6R)-2-carboxy-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-6-yl]-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

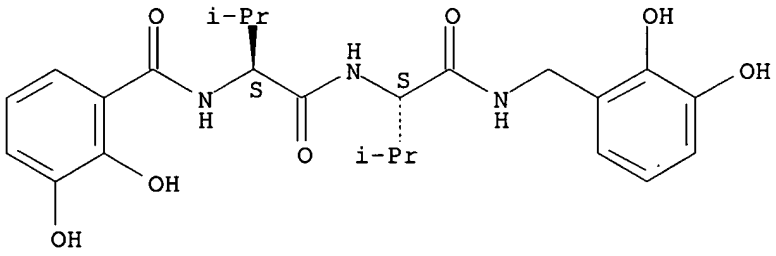
Absolute stereochemistry.



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 6 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2002:219733 CAPLUS
DN 137:72026
TI The fixation of linear versus loop-type peptidic structures by metal coordination: the coordination chemistry of Val-Val- and Val-Val-Val-bridged dicatechol ligands
AU Albrecht, Markus; Spiess, Oliver; Schneider, Matthias; Weis, Patrick
CS Institut fuer Organische Chemie, Universitaet Karlsruhe, Karlsruhe, D-76131, Germany
SO Chemical Communications (Cambridge, United Kingdom) (2002), (7), 786-787
CODEN: CHCOFS; ISSN: 1359-7345
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 137:72026
AB The Val-Val-bridged dicatechol ligand L1-H4 (I) forms triply-bridged dinuclear complexes with Ti(IV) ions, while the more flexible Val-Val-Val deriv. L2-H4 (II) leads to mixts. of complexes contg. species with a cyclic arrangement of the ligand. With [cis-MoO2]2+ however, a well-defined macrocycle [(L2)MoO2]2- is formed which possesses a loop-type structure in the peptidic part of the ligand.
IT **408349-66-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for prepn. of titanium valylvalyl linked dicatechol complex)
RN 408349-66-6 CAPLUS
CN L-Valinamide, N-(2,3-dihydroxybenzoyl)-L-valyl-N-[(2,3-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 7 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2002:90007 CAPLUS
DN 136:151439
TI Preparation of novel peptides as NS3-serine protease inhibitors of hepatitis C virus
IN Saksena, Anil K.; Girijavallabhan, Viyyoor Moopil; Bogen, Stephane L.; Lovey, Raymond G.; Jao, Edwin E.; Bennett, Frank; McCormick, Jinping L.; Wang, Haiyan; Pike, Russell E.; Liu, Yi-Tsung; Chan, Tin-Yau; Zhu, Zhaoning; Arasappan, Ashok; Chen, Kevin X.; Venkatraman, Srikanth; Parekh, Tejal N.; Pinto, Patrick A.; Santhanam, Bama; Njoroge, F. George; Ganguly, Ashit K.; Vaccaro, Henry A.; Kemp, Scott Jeffrey; Levy, Odile Esther; Lim-Wilby, Marguerita; Tamura, Susan Y.
PA Schering Corporation, USA; Corvas International, Inc.
SO PCT Int. Appl., 188 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002008187	A1	20020131	WO 2001-US22813	20010719
	WO 2002008187	C2	20030103		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NO, NZ, PL, PT, RO, RU, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2002160962	A1	20021031	US 2001-909012	20010719
	EP 1303487	A1	20030423	EP 2001-959041	20010719
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	NO 2003000271	A	20030318	NO 2003-271	20030120
PRAI	US 2000-220107P	P	20000721		
	WO 2001-US22813	W	20010719		

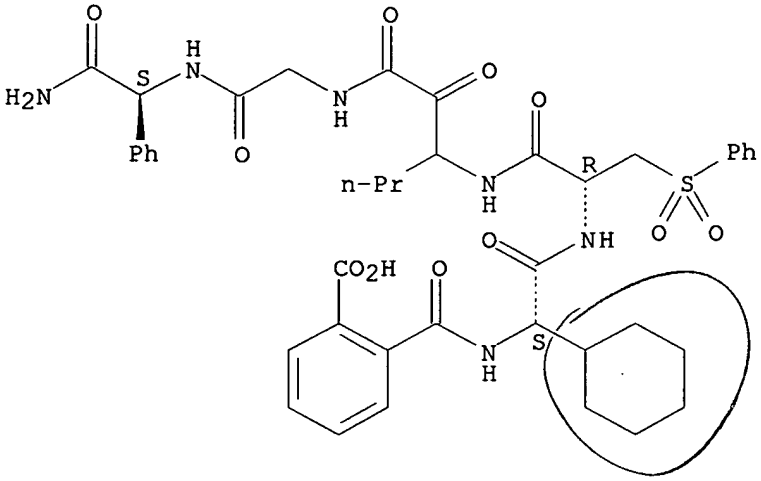
OS MARPAT 136:151439
AB Novel peptides I [G, J, Y = independently H, alkyl, alkyl-aryl, heteroalkyl, heteroaryl, aryl-heteroaryl, alkyl-heteroaryl, cycloalkyl, alkoxy, alkyl-aryloxy, aryloxy, heteroaryloxy, heterocycloalkyloxy, cycloalkyloxy, alkylamino, arylamino, alkyl-arylamino, arylamino, heteroarylamino, cycloalkylamino, and heterocycloalkylamino; Z = O, N, CH; W = null, CO, CS, SO2; R1 = COR5, B(OR)2; R5 = H, OH, OR8, NR9R10, CF3, C2F5, C3F7, CF2R6, R6, COR7; R7 = H, OH, OR8, CHR9R10, NR9R10; R6, R8-10 = independently H, alkyl, aryl, heteroalkyl, cycloalkyl, arylalkyl, peptide deriv., etc.; R, R2-4 = independently H, alkyl, alkenyl, cycloalkyl, heterocycloalkyl, alkoxy, aryloxy, alkylthio, arylthio, amino, amido, ester, carboxylic acid, carbamate, etc.] and their pharmaceutically salts which have hepatitis C virus (HCV) protease inhibitory activity were prepd. via soln. or solid-phase peptide coupling methods. Thus, peptide II was prepd. using solid-phase methods and showed a Ki value in the range of 0-100 nM for HCV protease inhibitory activity. This invention also discloses pharmaceutical compns. comprising such compds. as well as methods of using them to treat disorders assocd. with the HCV protease.
IT **393582-20-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel peptides as NS3-serine protease inhibitors of hepatitis C virus)

RN 393582-20-2 CAPLUS

CN Glycinamide, (2S)-N-(2-carboxybenzoyl)-2-cyclohexylglycyl-3-(phenylsulfonyl)-L-alanyl-3-amino-2-oxohexanoylglycyl-2-phenyl-, (2S)-(9CI) (CA INDEX NAME)

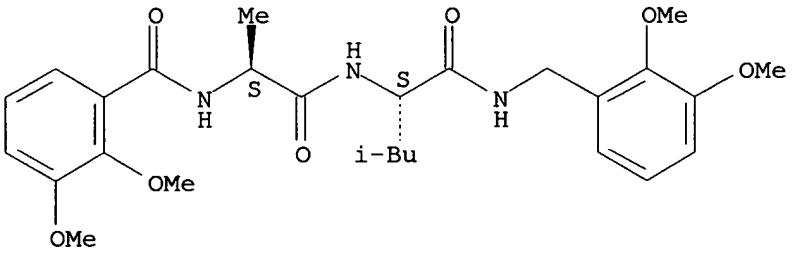
Absolute stereochemistry.



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

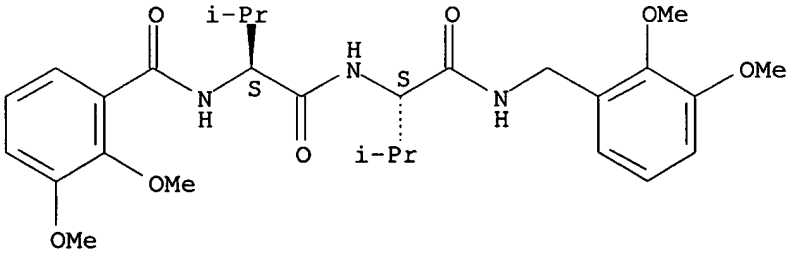
L27 ANSWER 8 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2002:48961 CAPLUS
DN 136:295078
TI Di-, tri- and tetrapeptide-linked dicatechol derivatives
AU Albrecht, Markus; Spiess, Oliver; Schneider, Matthias
CS Institut fur Organische Chemie, Universitat Karlsruhe, Karlsruhe, 76131, Germany
SO Synthesis (2002), (1), 126-132
CODEN: SYNTBF; ISSN: 0039-7881
PB Georg Thieme Verlag
DT Journal
LA English
AB Di-, tri- and tetrapeptide linked dicatechol derivs. are prepd. by subsequent coupling of 2,3-dimethoxybenzoic acid, peptides and 2,3-dimethoxybenzylamine using classical activating conditions (EDC/HOBt or DDC/HOSu). In the final step the Me ethers at the veratrol units are cleaved to afford the free catechol derivs. [I; Xxx-Yyy = Ala-Leu, (Val)2, (Leu)3, (Val)3, Ala-Val-Leu, (Phe-Leu)2], which are potential ligands for metal complexes with well defined fixed conformations at the peptide spacers.
IT **408349-44-0P 408349-49-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of peptide-linked dicatechol derivs.)
RN 408349-44-0 CAPLUS
CN L-Leucinamide, N-(2,3-dimethoxybenzoyl)-L-alanyl-N-[(2,3-dimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



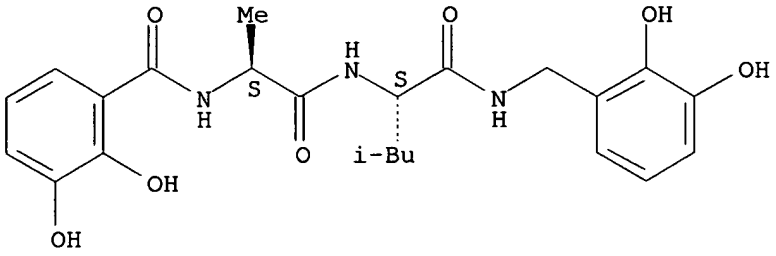
RN 408349-49-5 CAPLUS
CN L-Valinamide, N-(2,3-dimethoxybenzoyl)-L-valyl-N-[(2,3-dimethoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



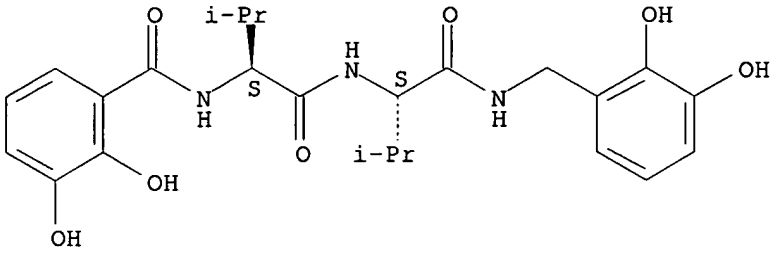
IT **408349-62-2P 408349-66-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptide-linked dicatechol derivs.)
RN 408349-62-2 CAPLUS
CN L-Leucinamide, N-(2,3-dihydroxybenzoyl)-L-alanyl-N-[(2,3-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 408349-66-6 CAPLUS
CN L-Valinamide, N-(2,3-dihydroxybenzoyl)-L-valyl-N-[(2,3-dihydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 9 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2001:906022 CAPLUS
DN 136:39535
TI Method for screening chromatographic adsorbents
IN Welch, Christopher J.; Protopopova, Marina; Ganapati, Bhat
PA USA
SO U.S. Pat. Appl. Publ., 23 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

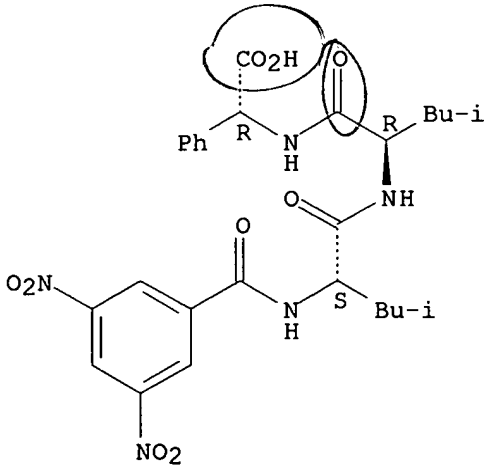
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2001050254	A1	20011213	US 1999-226941	19990108
US 6342160	B2	20020129		
PRAI US 1998-70887P	P	19980109		

AB A method for the rapid identification of a candidate selective sepn. material is described which involves the placing of small samples of the candidate material in an array of vials and adding a soln. of the analytes to be sepd. thereto. The soln. is allowed to interact or equilibrate and the distribution of the analytes in the solid or liq. phase is measured usually by gas or liq. chromatog. The identified candidate material with the greatest differential adsorption of the analytes is selected and used as an adsorbent for large scale sepn. The rapid screening of chromatog. adsorbents provides an efficient way of finding suitable absorbent materials for large scale sepns.

IT **220600-84-0D**, reaction products with aminopropylated silica
RL: ARG (Analytical reagent use); CST (Combinatorial study, unclassified); ANST (Analytical study); CMBI (Combinatorial study); USES (Uses)
(chromatog. adsorbent; combinatorial library-type screening method for chromatog. adsorbents)

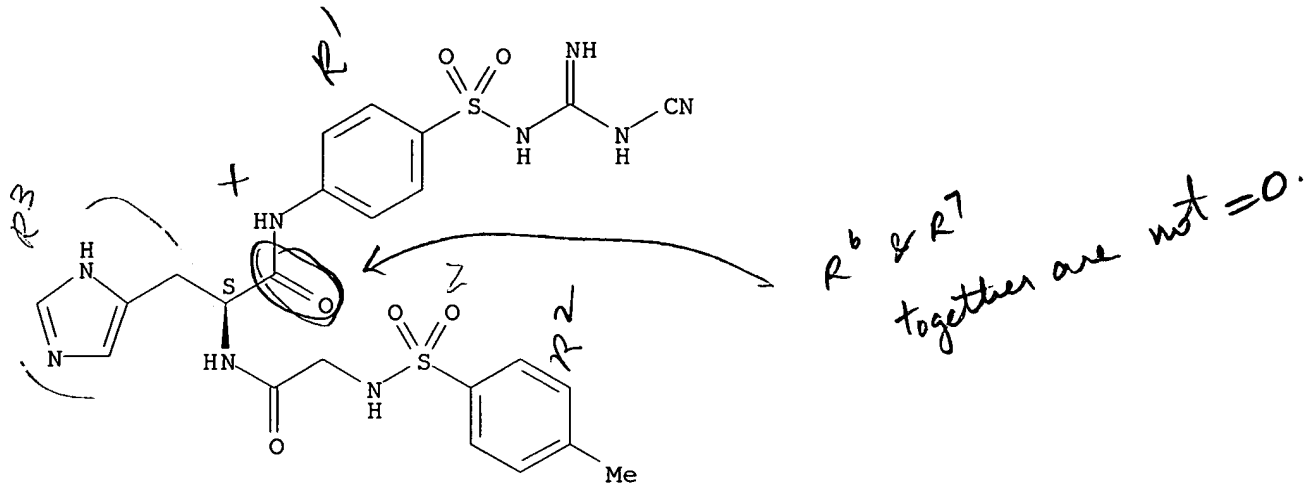
RN 220600-84-0 CAPLUS
CN Glycine, N-(3,5-dinitrobenzoyl)-L-leucyl-D-leucyl-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



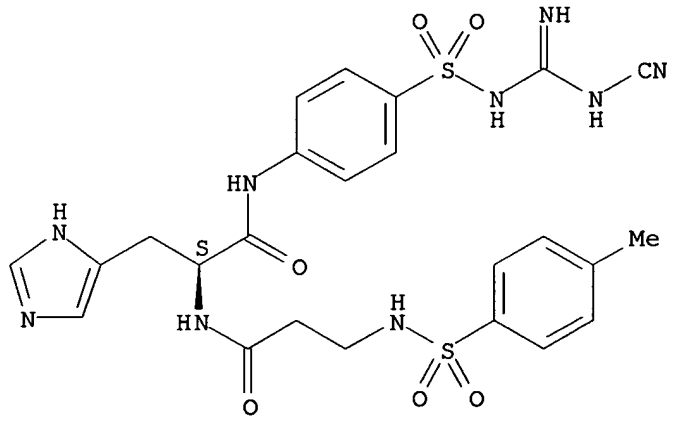
L27 ANSWER 10 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2001:271407 CAPLUS
DN 135:57729
TI Protease inhibitors, part 13: specific, weakly basic thrombin inhibitors incorporating sulfonyl dicyandiamide moieties in their structure
AU Clare, Brian W.; Scozzafava, Andrea; Supuran, Claudiu T.
CS Department of Chemistry, The University of Western Australia, Nedlands, 6009, Australia
SO Journal of Enzyme Inhibition (2001), 16(1), 1-13
CODEN: ENINEG; ISSN: 8755-5093
PB Harwood Academic Publishers
DT Journal
LA English
AB A series of compds. has been prepd. by reaction of dicyandiamide with alkyl/arylsulfonyl halides as well as arylsulfonyl isocyanates to locate a lead for obtaining weakly basic thrombin inhibitors with sulfonyl dicyandiamide moieties as the S1 anchoring group. The detected lead was sulfanilyl-dicyandiamide (KI of 3 .mu.M against thrombin, and 15 .mu.M against trypsin), which has been further derivatized at the 4-amino group by incorporating arylsulfonylureido as well as amino acyl/dipeptidyl groups protected at the amino terminal moiety with benzyloxycarbonyl or tosylureido moieties. The best compd. obtained (ts-D-Phe-Pro-sulfanilyl-dicyandiamide) showed inhibition consts. of 9 nM against thrombin and 1400 nM against trypsin. The pKa measurements showed that the new derivs. reported here do indeed possess a reduced basicity, with the pKa of the modified guanidine moieties in the range 7.9-8.3 pKa units. Mol. mechanics calcns. showed that the preferred tautomeric form of these compds. is of the type ArSO2N=C(NH2) NH-CN, probably allowing for the formation of favorable interaction between this new anchoring group and the active site amino acid residue Asp 189, crit. for substrate/inhibitor binding to this type of serine protease. Thus, the main finding of the present paper is that the sulfonyldicyandiamide group may constitute an interesting alternative for obtaining weakly basic, potent thrombin inhibitors, which bind with less affinity to trypsin.
IT **345916-26-9P 345916-27-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of specific, weakly basic thrombin inhibitors incorporating sulfonyl dicyandiamide moieties in their structure)
RN 345916-26-9 CAPLUS
CN L-Histidinamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-[4-[[[(cyanoamino)iminomethyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 345916-27-0 CAPLUS
CN L-Histidinamide, N-[(4-methylphenyl)sulfonyl]-.beta.-alanyl-N-[4-[[[(cyanoamino)iminomethyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

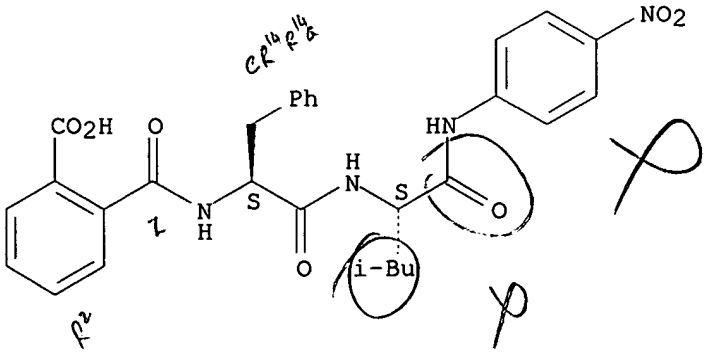
Absolute stereochemistry.



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 11 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2001:156312 CAPLUS
DN 134:322581
TI Insight into the Catalysis of Hydrolysis of Four Newly Synthesized Substrates by Papain: A Proton Inventory Study
AU Theodorou, Leonidas G.; Lymperopoulos, Kostas; Bieth, Joseph G.; Papamichael, Emmanuel M.
CS Department of Chemistry, Laboratory of Biochemistry, University of Ioannina, Ioannina, 451-10, Greece
SO Biochemistry (2001), 40(13), 3996-4004
CODEN: BICHAW; ISSN: 0006-2960
PB American Chemical Society
DT Journal
LA English
AB We synthesized the following four new peptide substrates, Suc-Phe-Leu-pNA, Suc-Phe-Leu-NMec, Suc-Phe-Leu-ONPh, and Pht-Phe-Leu-pNA, and we applied the proton inventory method to their hydrolysis by papain. Useful relationships between the rate consts. of the catalytic reaction have been established and contributed to the elucidation of the hydrolytic mechanism of papain. For all amide substrates, the parameter KS and the rate consts. k1, k-1, and k2 were estd. Moreover, it was found that kcat/Km = k1 for all four substrates, while two exchangeable hydrogenic sites, one in the ground state and another in the transition state, generate an inverse isotope effect during the reaction governed by this parameter. The proton inventories of both k2 and k3 are essentially linear, whatever the acyl moiety and/or the leaving group of the substrate. The proton inventories of KS are also essentially linear for all amide substrates, while the obsd. large isotope effect of about 3 to 9 originates from a single hydrogenic site in the product state. This latter, in agreement with both the small transition state fractionation factors found for kcat/Km (or k1) and the unit ground-state fractionation factors found for k2, argues for the formation of a tetrahedral adduct during the reaction governed by the k1 parameter. Furthermore, papain acts as a one-proton catalyst during acylation or deacylation, both of which proceed through similar concerted reaction pathways, where a nucleophilic attack is accompanied by the movement of one proton.
IT **286432-34-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(proton inventory study provides useful rate const. relationships for hydrolysis of dipeptide substrates by papain)
RN 286432-34-6 CAPLUS
CN L-Leucinamide, N-(2-carboxybenzoyl)-L-phenylalanyl-N-(4-nitrophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

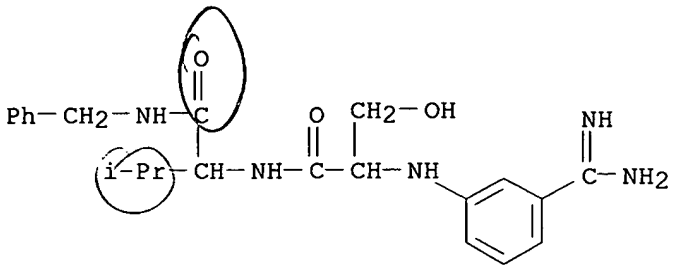


L27 ANSWER 12 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2001:152636 CAPLUS
DN 134:208135
TI Preparation of peptidomimetics as inhibitors of tryptase activity
IN Weber, Lutz; Fuchs, Thilo; Illgen, Katrin; Doemling, Alexander; Cappi, Michael; Nerdinger, Sven
PA Morphochem A.-G., Germany
SO PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001014320	A1	20010301	WO 2000-EP8238	20000823
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	DE 19939910	A1	20010301	DE 1999-19939910	19990823
	EP 1206444	A1	20020522	EP 2000-953198	20000823
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	JP 2003507450	T2	20030225	JP 2001-518410	20000823
	US 2002137687	A1	20020926	US 2002-81009	20020220
PRAI	DE 1999-19939910	A	19990823		
	WO 2000-EP8238	W	20000823		

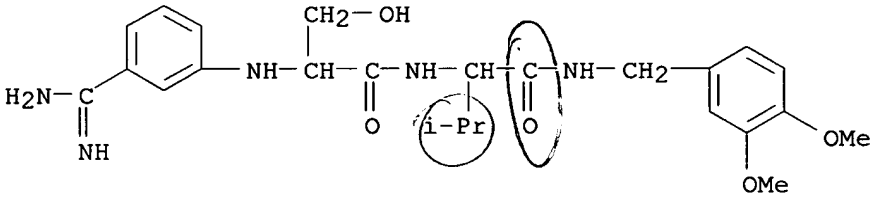
OS MARPAT 134:208135
AB Compds. X-Ar-NR3CHR4CONR8CHR5CONR6R7 [X is H2NC(:NH) or R1N:C(NH2), where R1 is OH, CO2R2, alkyl, aralkyl, aralkyloxy, or heteroalkyl and R2 is alkyl, heteroalkyl, carbocyclyl, heterocycloalkyl, aryl, heteroaryl, or aralkyl; Ar is arylene, heteroarylene, or aralkylene where X is directly attached to the arom. ring system; R3 is H, alkyl, heteroalkyl, or aralkyl; R4 is H, (un)substituted alkyl, heteroalkyl, carbocyclyl, heterocycloalkyl, aryl, heteroaryl, or aralkyl; R5 is H, alkyl, heteroalkyl, carbocyclyl, heterocycloalkyl, aryl, heteroaryl, or aralkyl; R6 and R7 are H, (un)substituted alkyl, heteroalkyl, carbocyclyl, or heterocycloalkyl; R8 is H, alkyl, heteroalkyl, carbocyclyl, heterocycloalkyl,aryl, heteroaryl or aralkyl] or a pharmaceutically acceptable salt, solvate, hydrate or formulation were prepd. as tryptase inhibitors. Thus, a soln. of glycolaldehyde, 3-aminobenzamidine dihydrochloride, and N-[2-(1H-indol-3-yl)ethyl]-3-methylbutanamide-2-isonitrile in methanol, allowed to react for 24 h at room temp. in a sealed vessel, afforded 2-{[2-({3-[amino(imino)methyl]phenyl}amino)-3-hydroxypropanoyl]amino}-N-[2-(1H-indol-3-yl)ethyl]-3-methylbutanamide hydrochloride, which showed IC50 = < 0.09 and 5 .mu.M for inhibition of tryptase and factor Xa, resp.
IT **328550-85-2P 328551-17-3P 328551-21-9P 328552-29-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of peptidomimetics as inhibitors of tryptase activity)

RN 328550-85-2 CAPLUS
CN Valinamide, N-[3-(aminoiminomethyl)phenyl]seryl-N-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)



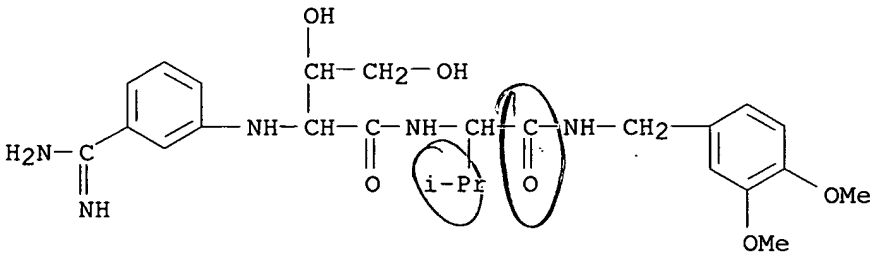
● x HCl

RN 328551-17-3 CAPLUS
CN Valinamide, N-[3-(aminoiminomethyl)phenyl]seryl-N-[(3,4-dimethoxyphenyl)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

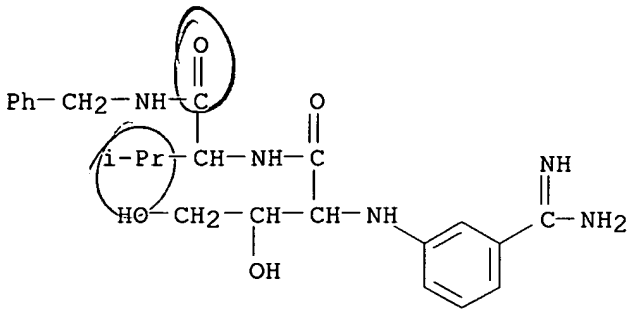
RN 328551-21-9 CAPLUS
CN Valinamide, N-[3-(aminoiminomethyl)phenyl]-3-hydroxyhomoseryl-N-[(3,4-dimethoxyphenyl)methyl]-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

RN 328552-29-0 CAPLUS

CN Valinamide, N-[3-(aminoiminomethyl)phenyl]-3-hydroxyhomoseryl-N-(phenylmethyl)-, hydrochloride (9CI) (CA INDEX NAME)



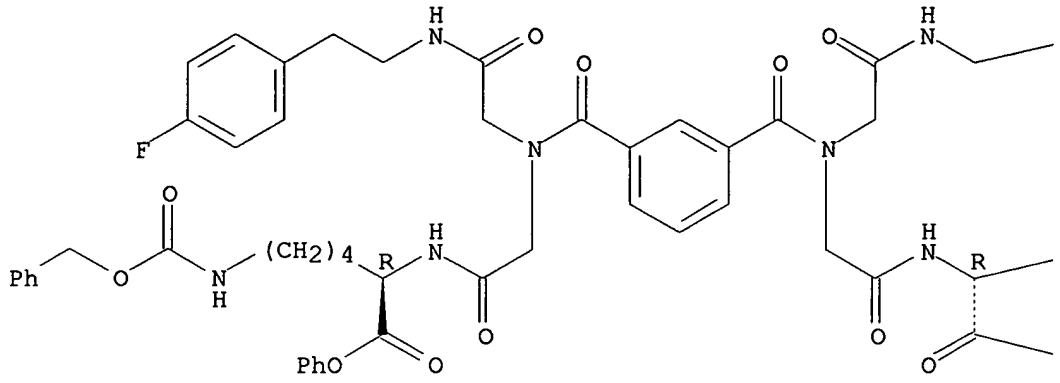
● x HCl

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

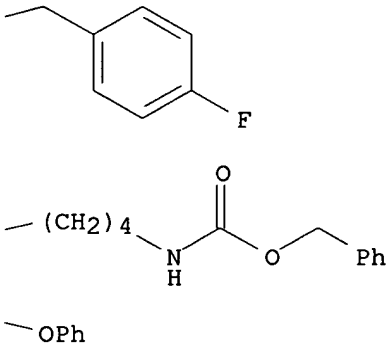
L27 ANSWER 13 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2001:61843 CAPLUS
DN 134:260866
TI Identification of a novel class of small-molecule antiangiogenic agents through the screening of combinatorial libraries which function by inhibiting the binding and localization of proteinase MMP2 to integrin .alpha.V.beta.3
AU Boger, Dale L.; Goldberg, Joel; Silletti, Steve; Kessler, Torsten; Cheresh, David A.
CS Departments of Chemistry Immunology and Vascular Biology, The Skaggs Institute for Chemical Biology The Scripps Research Institute, La Jolla, CA, 92037, USA
SO Journal of the American Chemical Society (2001), 123(7), 1280-1288
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 134:260866
AB The process of new blood vessel growth from existing vasculature, known as angiogenesis, is crit. to several pathol. conditions, most notably cancer. Both MMP2, which degrades the extracellular matrix (ECM), and integrin .alpha.V.beta.3, which contributes to endothelial cell attachment to the ECM, are critically involved in this process. Recent findings have shown that MMP2 is localized in an active form on the surface of invasive endothelial cells based on its ability to directly bind integrin .alpha.V.beta.3, suggesting that disrupting this protein-protein interaction may represent a new target for the development of angiogenesis inhibitors. The screening of small mol. libraries led to the identification of compds. which disrupt the MMP2-.alpha.V.beta.3 interaction in an in vitro binding assay. A prototypical inhibitor was further found to prevent the degrdn. of the protein matrix without directly inhibiting MMP2 activity or disrupting the binding of .alpha.V.beta.3 to its classical ECM ligand, vitronectin. The synthesis and screening of analogs and substructures of this lead compd. allowed the identification of requisite structural features for inhibition of MMP2 binding to .alpha.V.beta.3. This led to the synthesis of a more water-sol. deriv. which maintains the in vitro biol. properties and has potent antiangiogenic and antitumor activity in vivo, validating the target as one useful for therapeutic intervention.
IT **331714-18-2P**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(identification of novel class of small-mol. antiangiogenic agents through screening of combinatorial libraries)
RN 331714-18-2 CAPLUS
CN D-Lysine, 1,1'-(1,3-phenylenedicarbonyl)bis[N-[2-[[2-(4-fluorophenyl)ethyl]amino]-2-oxoethyl]glycyl-N6-[(phenylmethoxy)carbonyl]-, diphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 14 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2000:876774 CAPLUS
DN 134:37024
TI Factor VIIa inhibitors
IN Klingler, Otmar; Schudok, Manfred; Zoller, Gerhard; Heinelt, Uwe; Defossa, Elisabeth; Matter, Hans; Safar, Pavel
PA Aventis Pharma Deutschland G.m.b.H., Germany
SO Eur. Pat. Appl., 38 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 1059302	A1	20001213	EP 1999-111109	19990608
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	WO 2000075172	A2	20001214	WO 2000-EP4846	20000527
	WO 2000075172	A3	20010531		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	BR 2000011461	A	20020319	BR 2000-11461	20000527
	EP 1189929	A2	20020327	EP 2000-938691	20000527
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2003502294	T2	20030121	JP 2001-502453	20000527
	EE 200100662	A	20030415	EE 2001-662	20000527
	US 6500803	B1	20021231	US 2000-588651	20000607
	NO 2001006005	A	20020206	NO 2001-6005	20011207
PRAI	EP 1999-111109	A	19990608		
	WO 2000-EP4846	W	20000527		

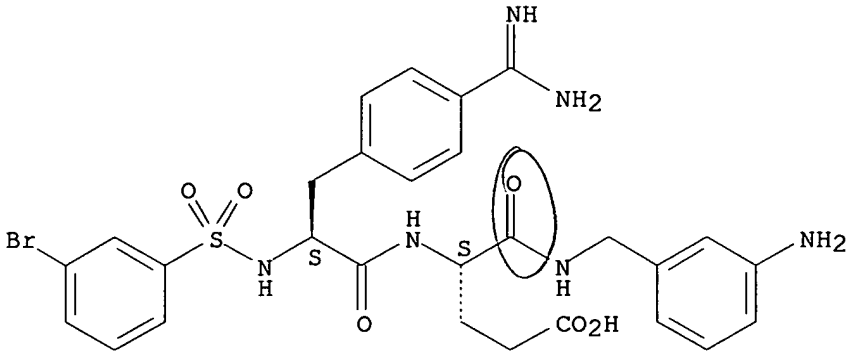
OS MARPAT 134:37024
AB The present invention relates to compds. of the formula (I; where R1 = alkylCO arylCO, alkylSO2 or arylSO2, etc.; R2 = H, alkyl, aryl, heterocycle, etc.; R91, R92 and R93 which are independent of each other and = alkyl, aryl, heterocycle, etc.; R94 = alkyl, aryl, amino, etc.; R95 = amidino, guanidino, alkyloxycarbonylamidino, etc.; R96 and R97 = H, alkyl, aryl, alkyloxycarbonyl, etc.; r = 0-3; s = 0-4 and t= 0-2). The compds. of the formula I are valuable pharmacol. active compds. They exhibit a strong antithrombotic effect and are suitable, for example, for the therapy and prophylaxis of thromboembolic diseases or restenoses. They are reversible inhibitors of the blood clotting enzyme factor VIIa and can in general be applied in conditions in which an undesired activity of factor VIIa is present or for the cure or prevention of which an inhibition of factor VIIa is intended. The invention furthermore relates to processes for the prepn. of compds. of the formula I, their use, in particular as active ingredients in pharmaceuticals, and pharmaceutical prepns. comprising them.
IT **312581-20-7P 312581-21-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)
(factor VIIa inhibitors as antithrombotics in relation to prepn. of peptide-like compds.)

RN 312581-20-7 CAPLUS

CN L-.alpha.-Glutamine, 4-(aminoiminomethyl)-N-[(3-bromophenyl)sulfonyl]-L-phenylalanyl-N-[(3-aminophenyl)methyl]- (9CI) (CA INDEX NAME)

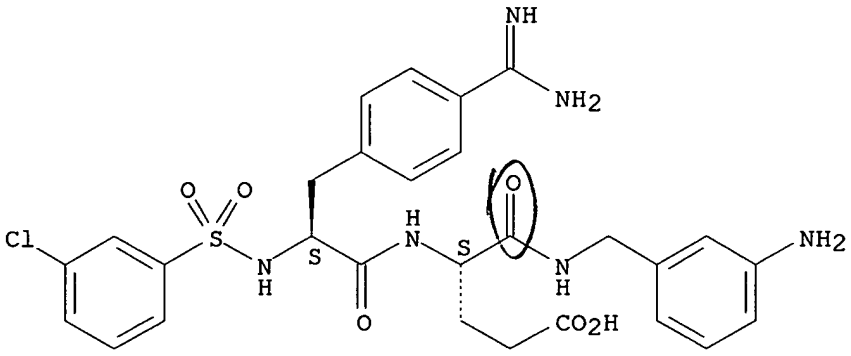
Absolute stereochemistry.



RN 312581-21-8 CAPLUS

CN L-.alpha.-Glutamine, 4-(aminoiminomethyl)-N-[(3-chlorophenyl)sulfonyl]-L-phenylalanyl-N-[(3-aminophenyl)methyl]- (9CI) (CA INDEX NAME)

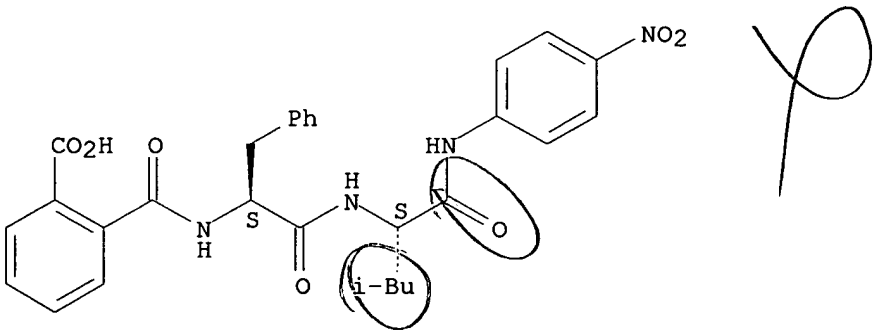
Absolute stereochemistry.



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 15 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 2000:243308 CAPLUS
DN 133:131586
TI Detection of S1-P1 and S3-P3 interactions between papain and four synthetic substrates
AU Papamichael, Emmanuel M.; Roustas, Michael K.; Bieth, Joseph G.
CS Sector of Organic Chemistry and Biochemistry, Department of Chemistry, University of Ioannina, Ioannina, 45110, Greece
SO Brazilian Archives of Biology and Technology (1999), 42(3), 277-280
CODEN: BABTFC; ISSN: 1516-8913
PB Instituto de Tecnologia do Parana
DT Journal
LA English
AB In this study, the S1-P1 and S3-P3 interactions between papain and four synthetic peptide substrates were found to be important. The values of Km were estd. as to be practically identical between these substrates; this latter is supporting the conclusions obtained by considering the estd. values of other kinetic parameters. Nevertheless, based on the estd. kcat and/or kcat/Km parameters of the substrates, we concluded that an arom. ring at the P3 position, and a pos. charged side chain of the residue at the P1 position of the synthetic substrates were favored considerably for interaction with papain.
IT **286432-34-6**
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(detection of S1-P1 and S3-P3 interactions between papain and four synthetic substrates)
RN 286432-34-6 CAPLUS
CN L-Leucinamide, N-(2-carboxybenzoyl)-L-phenylalanyl-N-(4-nitrophenyl)-(9CI) (CA INDEX NAME)

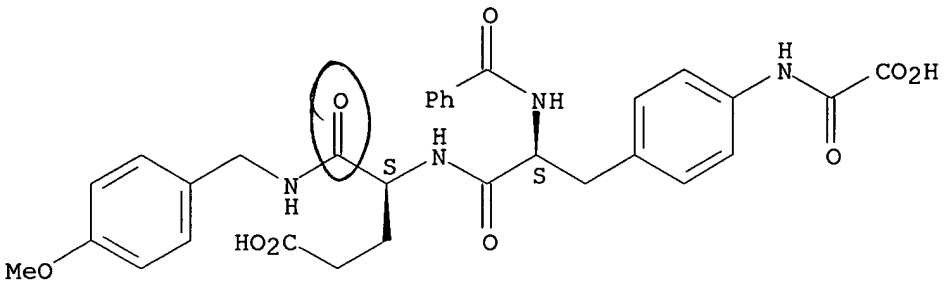
Absolute stereochemistry.



RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 16 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1999:261309 CAPLUS
DN 131:67637
TI Ligands for the Tyrosine Kinase p56lck SH2 Domain: Discovery of Potent Dipeptide Derivatives with Monocharged, Nonhydrolyzable Phosphate Replacements
AU Beaulieu, Pierre L.; Cameron, Dale R.; Ferland, Jean-Marie; Gauthier, Jean; Ghiro, Elise; Gillard, James; Gorys, Vida; Poirier, Martin; Rancourt, Jean; Wernic, Dominik; Llinas-Brunet, Montse; Betageri, Raj; Cardozo, Mario; Hickey, Eugene R.; Ingraham, Richard; Jakes, Scott; Kabcenell, Alisa; Kirrane, Tom; Lukas, Susan; Patel, Usha; Proudfoot, John; Sharma, Rajiv; Tong, Liang; Moss, Neil
CS Bio-Mega Research Division, Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S 2G5, Can.
SO Journal of Medicinal Chemistry (1999), 42(10), 1757-1766
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB P56lck is a member of the src family of tyrosine kinases. Through modular binding units called SH2 domains, p56lck promotes phosphotyrosine-dependent protein-protein interactions and plays a crit. role in signal transduction events that lead to T-cell activation. Starting from the phosphorylated dipeptide (I), a high-affinity ligand for the p56lck SH2 domain, novel dipeptides were designed that contain monocharged, nonhydrolyzable phosphate group replacements and bind to the protein with KD's in the low micromolar range. Replacement of the phosphate group in phosphotyrosine-contg. sequences by a (R/S)-hydroxyacetic or an oxamic acid moiety leads to hydrolytically stable, monocharged ligands, with 83- and 233-fold decreases in potency, resp. This loss in binding affinity can be partially compensated for by incorporating large lipophilic groups at the inhibitor N-terminus. These groups provide up to 13-fold increases in potency depending on the nature of the phosphate replacement. The discovery of potent (2-3 .mu.M), hydrolytically stable dipeptide derivs., bearing only two charges at physiol. pH, represents a significant step toward the discovery of compds. with cellular activity and the development of novel therapeutics for conditions assocd. with undesired T-cell proliferation.
IT **229171-44-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(design and prepn. of dipeptide derivs. as ligands for binding to tyrosine kinase p56lck SH2 domain)
RN 229171-44-2 CAPLUS
CN L-.alpha.-Glutamine, N-benzoyl-4-[(carboxycarbonyl)amino]-L-phenylalanyl-N-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

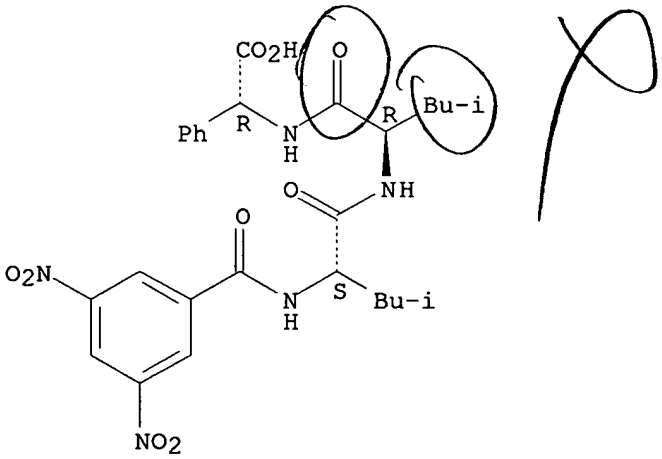
Absolute stereochemistry.



RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 17 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1999:37246 CAPLUS
DN 130:182752
TI Silica-based solid phase synthesis of chiral stationary phases
AU Welch, Christopher J.; Bhat, Ganapati; Protopopova, Marina N.
CS Regis Technologies, Inc., Morton Grove, IL, 60053, USA
SO Enantiomer (1998), 3(6), 463-469
CODEN: EANTE2; ISSN: 1024-2430
PB Gordon & Breach Science Publishers
DT Journal
LA English
AB An approach to the prepn. of chiral stationary phases (CSPs) employing silica-based solid phase peptide synthesis is described. A no. of 3,5-dinitrobenzoyl dipeptide and tripeptide CSPs were prepd. using a modified solid phase synthesis protocol. Evaluation of these CSPs reveals some interesting properties and suggests that the technique of solid phase CSP synthesis may be useful for prepn. of combinatorial CSP libraries.
IT **220600-84-0DP**, amide with aminopropyl silica gel
RL: NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(silica-based solid phase synthesis of dinitrobenzoyl peptide chiral stationary phases)
RN 220600-84-0 CAPLUS
CN Glycine, N-(3,5-dinitrobenzoyl)-L-leucyl-D-leucyl-2-phenyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



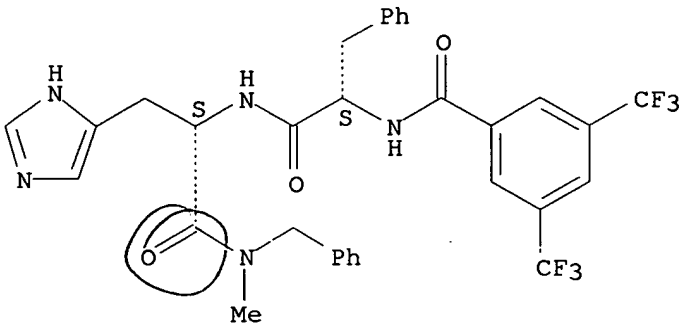
RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 18 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1998:724213 CAPLUS
DN 130:38715
TI Preparation of substituted benzamides and their use for treatment of respiratory disorders, headache, and emesis
IN Sakurada, Tsukasa; Sasaki, Jun; Oba, Masataka; Matsumura, Yasushi
PA Asahi Glass Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 10298197	A2	19981110	JP 1997-109581	19970425
PRAI JP 1997-109581		19970425		

OS MARPAT 130:38715
AB Substituted benzamides I [A = CO, CH2; B = NR3, O, S, CH2; R1, R2 = H, OH, halo, lower (halo)alkyl, etc.; R4, R5 = H, halo, lower alkyl, alkoxy; R6 = H, halo, alkyl, CONR7R8, CO2R9, COR10; X = H, halo, lower (halo)alkyl, alkoxy; n = 0-3; R3 = H, halo, lower alkyl, alkoxy; R7-R10 = H, lower alkyl, aralkyl, aryl; except a case where A = CO, B = NH, R1 = R2 = CF3, R4 = R5 = X = H, R6 = CONH2, and n = 1] or their salts are prepd. The benzamides are antagonists of the substance P/NK-1 receptor interaction (no data). Crude N-tert-butoxycarbonylphenylalanylhistamine (3 g) was deprotected by F3CCO2H and treated with 3,5-bis(trifluoromethyl)benzoic acid, HBTU, and HOBT in DMF to give 130 mg N-3,5-bis(trifluoromethyl)benzoylphenylalanylhistamine.
IT **216597-53-4P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of substituted benzamides for treatment of respiration disorders, headache, and emesis)
RN 216597-53-4 CAPLUS
CN L-Histidinamide, N-[3,5-bis(trifluoromethyl)benzoyl]-L-phenylalanyl-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 19 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1998:352862 CAPLUS
DN 129:41413
TI Preparation of N-aryl- and N-heteroaryl dipeptides for inhibiting .beta.-amyloid peptide release
IN Audia, James E.; Folmer, Beverly K.; John, Varghese; Latimer, Lee H.; Nissen, Jeffrey S.; Porter, Warren J.; Thorsett, Eugene D.; Wu, Jing
PA Athena Neurosciences, Inc., USA; Eli Lilly & Co.; Audia, James E.; Folmer, Beverly K.; John, Varghese; Latimer, Lee H.; Nissen, Jeffrey S.; Porter, Warren J.; Thorsett, Eugene D.; Wu, Jing
SO PCT Int. Appl., 131 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9822493	A2	19980528	WO 1997-US18704	19971120
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9853543	A1	19980610	AU 1998-53543	19971120
	EP 942923	A2	19990922	EP 1997-950576	19971120
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	CN 1237978	A	19991208	CN 1997-199776	19971120
	BR 9714358	A	20000321	BR 1997-14358	19971120
	NZ 335157	A	20010126	NZ 1997-335157	19971120
	JP 2001519769	T2	20011023	JP 1998-523649	19971120
	US 6096782	A	20000801	US 1997-976191	19971121
	US 2001020097	A1	20010906	US 1999-280966	19990330
	US 6495693	B2	20021217		
	MX 9904527	A	20000731	MX 1999-4527	19990514
	NO 9902426	A	19990630	NO 1999-2426	19990520
PRAI	US 1996-755334	A	19961122		
	US 1996-77175P	P	19961122		
	WO 1997-US18704	W	19971120		
	US 1997-976191	A1	19971121		

OS MARPAT 129:41413
AB Disclosed are title compds. I [R1 = (un)substituted Ph, (un)substituted 2-naphthyl, (un)substituted heteroaryl; R2 = H, C1-4 alkyl, C1-4 alkoxy, C1-4 alkylthio, (un)substituted aryl, (un)substituted heteroaryl; R3 = (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, aryl, cycloalkyl, cycloalkenyl, heteroaryl, heterocyclyl; X = CO-Y; Y = (un)substituted alkyl, (un)substituted alkoxy, (un)substituted alkylthio, OH, aryl, heteroaryl, heterocyclyl, (un)substituted amino; with provisos] which inhibit .beta.-amyloid peptide release and/or its synthesis, and, accordingly, have utility in treating Alzheimer's disease. Also disclosed are pharmaceutical compns. comprising a compd. which inhibits .beta.-amyloid peptide release and/or its synthesis as well as methods for treating Alzheimer's disease both prophylactically and therapeutically with such pharmaceutical compns. Thus, substitution of 3,4-dichloroaniline with 2-chloropropionic acid gave N-(3,4-

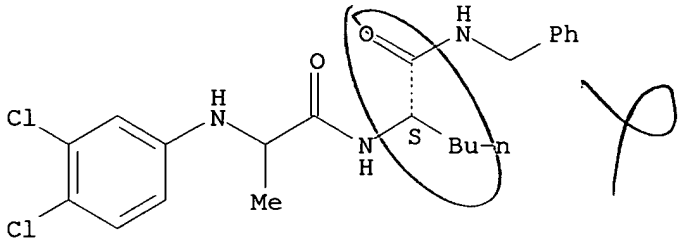
dichlorophenyl)-DL-alanine, which underwent peptide coupling with L-valine Me ester hydrochloride to give desired title compd. 3,4-Cl2C6H3-DL-Ala-Val-OMe.

IT **208331-15-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-aryl- and N-heteroaryl dipeptides for inhibiting .beta.-amyloid peptide release)

RN 208331-15-1 CAPLUS

CN L-Norleucinamide, N-(3,4-dichlorophenyl)alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

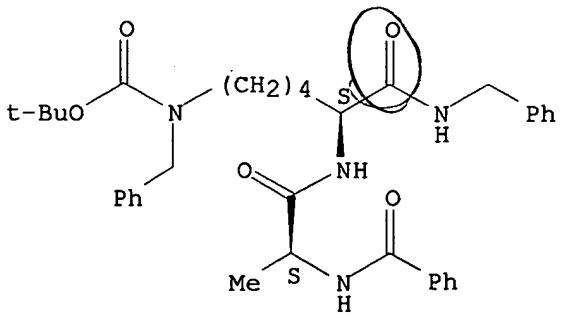


L27 ANSWER 20 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1998:323147 CAPLUS
DN 129:4650
TI Preparation of combinatorial libraries of cyclic urea and thiourea derivatives having antimicrobial and opioid receptor ligand activity.
IN Nefzi, Adel; Ostresh, John M.; Houghten, Richard
PA Trega Biosciences, Inc., USA
SO PCT Int. Appl., 85 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9819693	A1	19980514	WO 1997-US19945	19971105
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5786448	A	19980728	US 1996-745793	19961107
AU 9852433	A1	19980529	AU 1998-52433	19971105
PRAI US 1996-745793	A	19961107		
WO 1997-US19945	W	19971105		

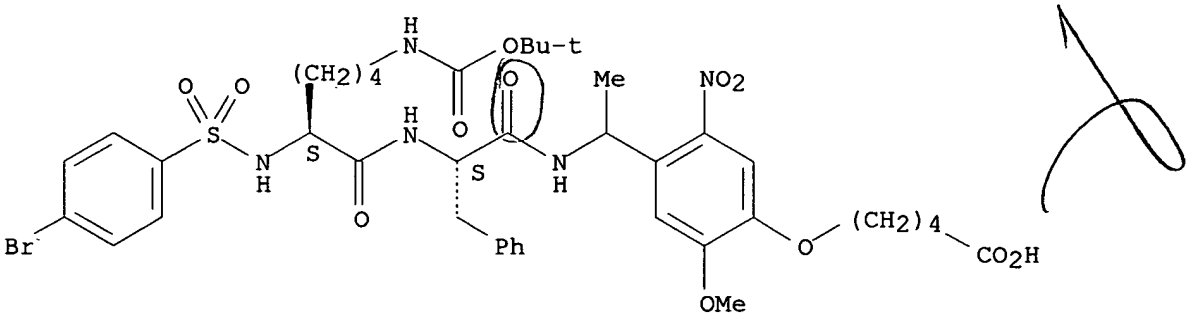
OS MARPAT 129:4650
AB A combinatorial library comprising .gtoreq.2 cyclic ureas [I; R1, R3 = H, (substituted) alkyl, phenylalkyl, Ph, cycloalkyl; R2 = alkyl, alkenyl, (substituted) PhCH2, naphthylmethyl; R4 = alkenyl, (substituted) alkyl, cycloalkyl, phenylalkyl, phenylalkenyl; X = O, S; n = 1, 2], is claimed. Ca 160 I pools were prepd. using solid phase techniques on MBHA resin; all pools of N-benzyl aminocyclic thioureas tested showed antimicrobial and .mu.- and .kappa.-receptor binding activity.
IT **207515-01-3D**, resin-bound
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of combinatorial libraries of cyclic urea and thiourea derivs. having antimicrobial and opioid receptor ligand activity)
RN 207515-01-3 CAPLUS
CN L-Lysinamide, N-benzoyl-L-alanyl-N6-[(1,1-dimethylethoxy)carbonyl]-N,N6-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 21 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1997:558873 CAPLUS
DN 127:191051
TI Photolytic Mass Laddering for Fast Characterization of Oligomers on Single Resin Beads
AU Burgess, Kevin; Martinez, Carlos I.; Russell, David H.; Shin, Hunwoo; Zhang, Alex J.
CS Department of Chemistry, Texas A+M University, College Station, TX, 77843-3255, USA
SO Journal of Organic Chemistry (1997), 62(17), 5662-5663
CODEN: JOCEAH; ISSN: 0022-3263
PB American Chemical Society
DT Journal
LA English
AB A photolytic mass-laddering technique for detg. peptide sequences attached to resin supports is described. A split synthesis is performed such that most of the growing oligomer on the resin bead consists of the unperturbed sequence, and a small fraction has a photolabile group, e.g. I (Boc = Me3CO2C), inserted before each of the coupling steps. On irradn., an isolated bead generates fragments of incrementally different mol. masses. Mass spectral anal. of the material liberated is used to deduce the sequence form the mol. mass differences. Isotopic distribution of the bromine isomers in the heavy part of the linker gives 1:1 mol. mass distributions for peaks contg. this fragment, allowing them to be easily differentiated from background signals.
IT **194143-45-8P 194143-49-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of photolabile group for rapid characterization of resin-bound peptides by mass laddering)
RN 194143-45-8 CAPLUS
CN L-Phenylalaninamide, N2-[(4-bromophenyl)sulfonyl]-N6-[(1,1-dimethylethoxy)carbonyl]-L-lysyl-N-[1-[4-(4-carboxybutoxy)-5-methoxy-2-nitrophenyl]ethyl]- (9CI) (CA INDEX NAME)

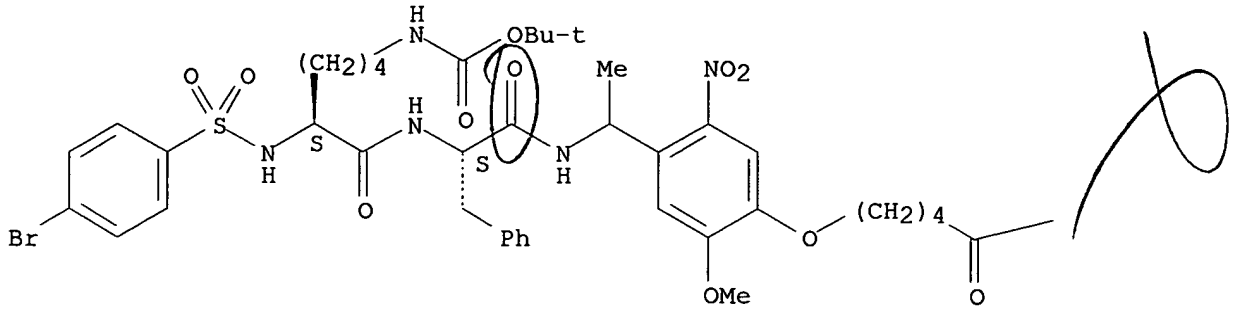
Absolute stereochemistry.



RN 194143-49-2 CAPLUS
CN L-Phenylalaninamide, N2-[(4-bromophenyl)sulfonyl]-N6-[(1,1-dimethylethoxy)carbonyl]-L-lysyl-N-[1-[5-methoxy-4-[(5-methoxy-5-oxopentyl)oxy]-2-nitrophenyl]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

File Copy

L27 ANSWER 22 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1997:290093 CAPLUS
DN 126:264011
TI Preparation of meta-guanidine, urea, thiourea or azacyclic amino benzoic acid derivatives as integrin antagonists
IN Ruminski, Peter Gerrard; Clare, Michael; Collins, Paul Waddell; Desai, Bipinchandra Nanubhai; Lindmark, Richard John; Rico, Joseph Gerace; Rogers, Thomas Edward; Russell, Mark Andrew; et al.
PA G.D. Searle & Co., USA; Ruminski, Peter Gerrard; Clare, Michael; Collins, Paul Waddell; Desai, Bipinchandra Nanubhai; Lindmark, Richard, John
SO PCT Int. Appl., 930 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9708145	A1	19970306	WO 1996-US13500	19960827
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
	CA 2230209	AA	19970306	CA 1996-2230209	19960827
	AU 9671039	A1	19970319	AU 1996-71039	19960827
	AU 702487	B2	19990225		
	EP 850221	A1	19980701	EP 1996-932142	19960827
	EP 850221	B1	20010718		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	CN 1201454	A	19981209	CN 1996-197911	19960827
	CN 1085980	B	20020605		
	BR 9610422	A	19990713	BR 1996-10422	19960827
	JP 11510814	T2	19990921	JP 1996-510397	19960827
	IL 123164	A1	20010319	IL 1996-123164	19960827
	AT 203234	E	20010815	AT 1996-932142	19960827
	ES 2161373	T3	20011201	ES 1996-932142	19960827
	RU 2196769	C2	20030120	RU 1998-105408	19960827
	NO 9800817	A	19980424	NO 1998-817	19980226
	HK 1021532	A1	20020208	HK 1998-114666	19981228
PRAI	US 1995-3277P	P	19950830		
	WO 1996-US13500	W	19960827		

OS MARPAT 126:264011
AB The title compds. I [A = (un)substituted ureido, guanidino, etc. (generic structures given); Z1 = H, alkyl, OH, alkoxy, halo, (di)(alkyl)amino, aryl, etc.; V = NR6; R6 = H, alkyl, etc.; or YR6 forms a 4- to 12-membered [illegible]-N-contg. ring; Y, Y3, Z, Z3 = H, alkyl, aryl, cycloalkyl; or YZ or Y3Z3 form cycloalkyl; n = 1-3; t = 0-2; p = 0-3; R = XR3; X = O, S, NH, etc.; R3 = H, alkyl, etc.; R1 = H, alkyl, alkenyl, etc.; R11 = H, alkyl, aralkyl, etc.] are prepd. For example, m-nitrohippuric acid was subjected to a sequence of (1) amidation with Et 3-amino-3-(3-pyridyl)propanoate-2HCl; (2) hydrogenation of the nitro group; (3) reaction of the formed amine with benzyl isocyanate; and (4) alk. sapon. of the ester, to give title compd. II, isolated as the CF3CO2H or HCl salt. In an in vitro assay for antagonism of human vitronectin receptor (.alpha.V.beta.3), the title compd. II.HCl bound with an IC50 of 0.86 nM.
IT **188804-85-5P 188805-16-5P**

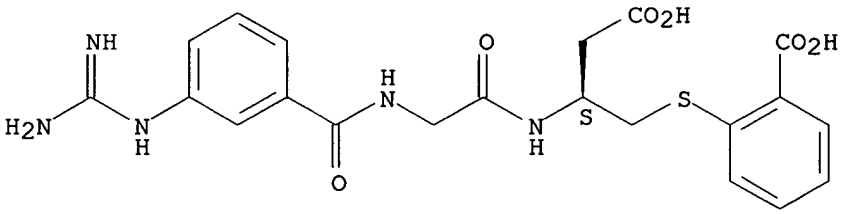
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of meta-guanidino, -ureido, -thioureido, or -azacyclic-amino benzoic acid derivs. as integrin antagonists)

RN 188804-85-5 CAPLUS
CN Benzoic acid, 2-[[2-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-3-carboxypropyl]thio]-, (S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

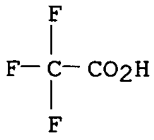
CRN 188804-84-4
CMF C21 H23 N5 O6 S

Absolute stereochemistry.



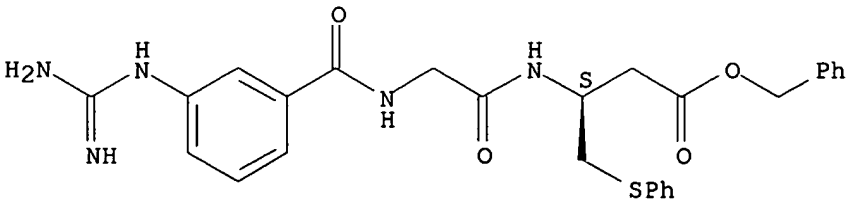
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 188805-16-5 CAPLUS
CN Butanoic acid, 3-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-4-(phenylthio)-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

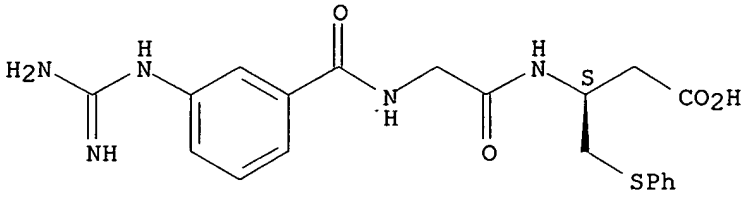


IT **188804-78-6P 188804-79-7P 188804-82-2P**

188804-83-3P 188804-84-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of meta-guanidino, -ureido, -thioureido, or -azacyclic-amino benzoic acid derivs. as integrin antagonists)

RN 188804-78-6 CAPLUS
CN Butanoic acid, 3-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-4-(phenylthio)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

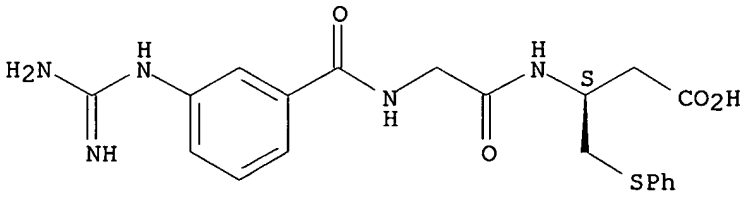


RN 188804-79-7 CAPLUS
CN Butanoic acid, 3-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-4-(phenylthio)-, (S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

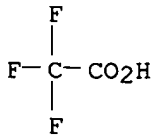
CRN 188804-78-6
CMF C20 H23 N5 O4 S

Absolute stereochemistry.



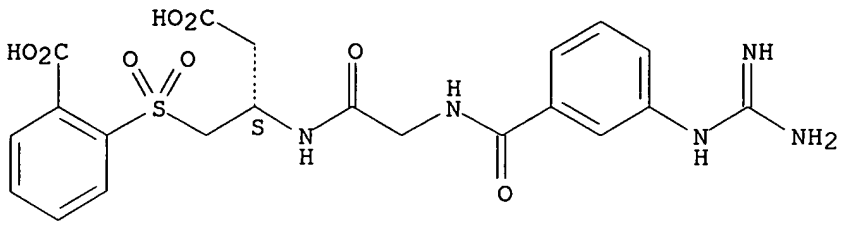
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 188804-82-2 CAPLUS
CN Benzoic acid, 2-[[2-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-3-carboxypropyl]sulfonyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

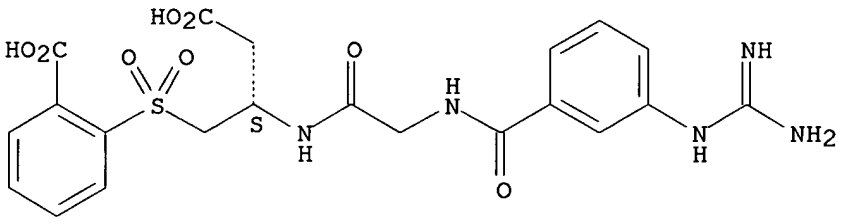


RN 188804-83-3 CAPLUS
CN Benzoic acid, 2-[[2-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-3-carboxypropyl]sulfonyl]-, (S)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

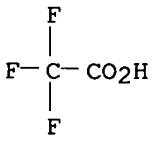
CRN 188804-82-2
CMF C21 H23 N5 O8 S

Absolute stereochemistry.



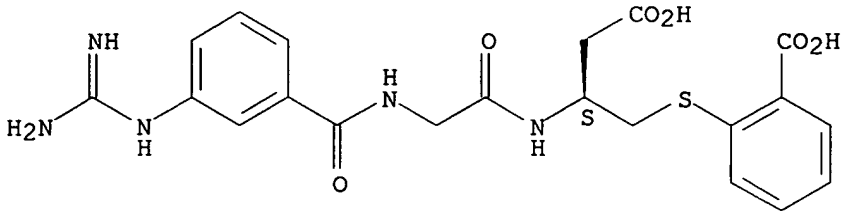
CM 2

CRN 76-05-1
CMF C2 H F3 O2



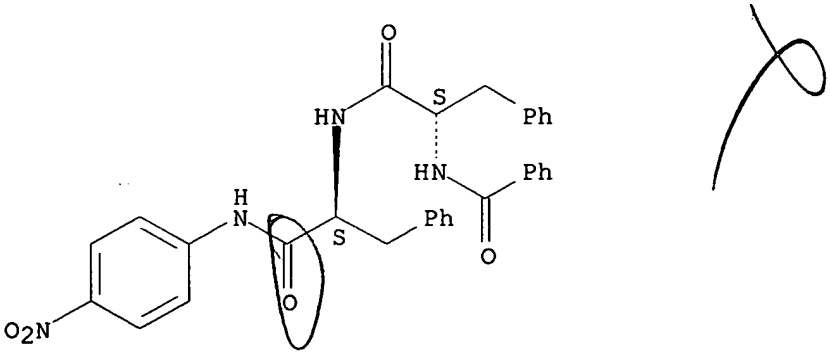
RN 188804-84-4 CAPLUS
CN Benzoic acid, 2-[[2-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-3-carboxypropyl]thio]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


NH
H2N
N
H
H
N
O
O
N
H
CO2H
S
S
CO2H

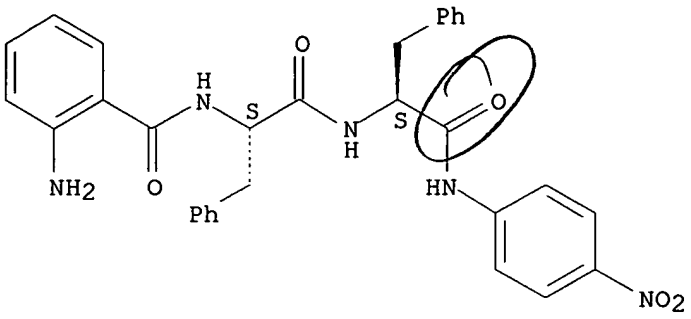
L27 ANSWER 23 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1997:248791 CAPLUS
DN 126:327291
TI Design of kallidin-releasing tissue kallikrein inhibitors based on the specificities of the enzyme's binding subsites
AU Portaro, Fernanda C. V.; Cezari, Maria H. S.; Juliano, Maria A.; Juliano, Luiz; Walmsley, Adrian R.; Prado, Eline S.
CS Department Biophysics, Universidade Federal Sao Paulo-Escola Paulista Medicina, Sao Paulo, 04044-020, Brazil
SO Biochemical Journal (1997), 323(1), 161-171
CODEN: BIJOAK; ISSN: 0264-6021
PB Portland Press
DT Journal
LA English
AB Tissue kallikrein inhibitors were derived by selectively replacing residues in N.alpha.-substituted arginine- or phenylalanine-pNA (where pNA is p-nitroanilide), and in peptide substrates for these enzymes. Phenylacetyl-Arg-pNA was an efficient inhibitor of human tissue kallikrein (Ki 0.4 .mu.M) and was neither a substrate nor an inhibitor of plasma kallikrein. The peptide inhibitors having phenylalanine as the P1 residue behaved as specific inhibitors for kallidin-releasing tissue kallikreins, whereas plasma kallikrein showed high affinity for inhibitors contg. (p-nitro)phenylalanine at the same position. The Ki value of the most potent inhibitor developed, Abz-Phe-Arg-Arg-Pro-Arg-EDDnp [where Abz is o-aminobenzoyl and EDDnp is N-(2,4-dinitrophenyl)-ethylenediamine], was 0.08 .mu.M for human tissue kallikrein. Progress curve analyses of the inhibition of human tissue kallikrein by benzoyl-Arg-pNA and phenylacetyl-Phe-Ser-Arg-EDDnp indicated a single-step mechanism for reversible formation of the enzyme-inhibitor complex.
IT **179166-91-7 189621-42-9 189621-43-0 189621-44-1 189621-45-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(design of kallidin-releasing tissue kallikrein inhibitors based on the specificities of the enzyme's binding subsites)
RN 179166-91-7 CAPLUS
CN L-Phenylalaninamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



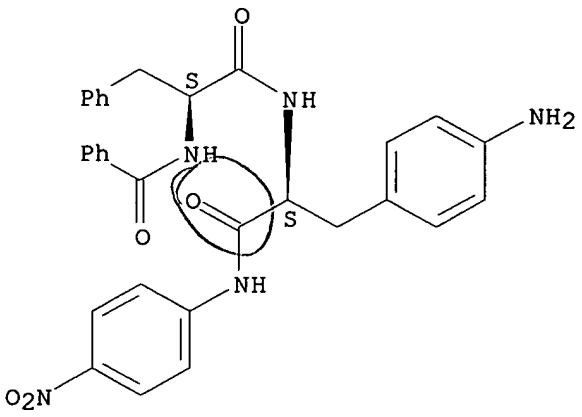
RN 189621-42-9 CAPLUS
CN L-Phenylalaninamide, N-(2-aminobenzoyl)-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



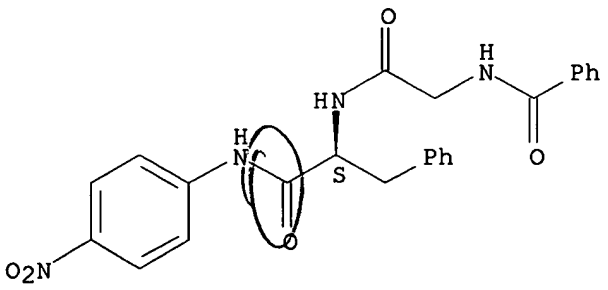
RN 189621-43-0 CAPLUS
CN L-Phenylalaninamide, N-benzoyl-L-phenylalanyl-4-amino-N-(4-nitrophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 189621-44-1 CAPLUS
CN L-Phenylalaninamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

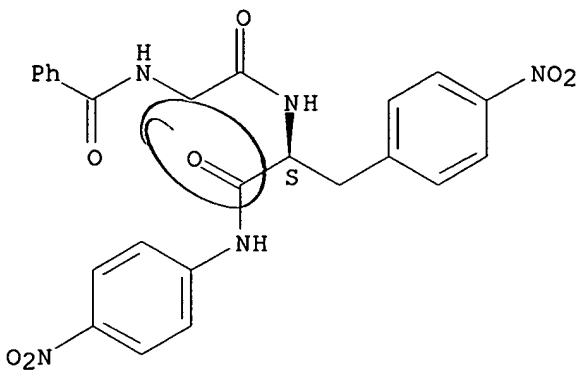
Absolute stereochemistry.



RN 189621-45-2 CAPLUS

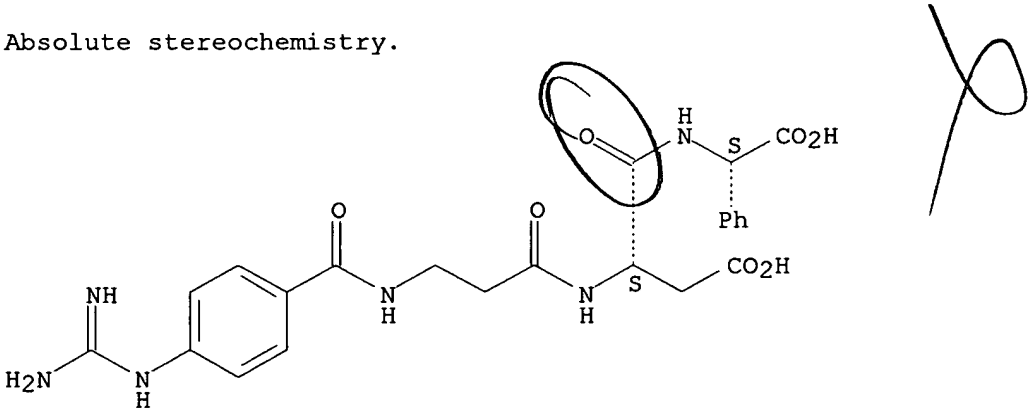
CN L-Phenylalaninamide, N-benzoylglycyl-4-nitro-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 24 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1996:696128 CAPLUS
DN 126:14337
TI New RGD peptide mimetics as efficient inhibitors of platelet aggregation
AU Chakravarty, S.; Dong, Q.; Ojima, I.
CS Department Chemistry, State University New York, Stony Brook, NY, 11794, USA
SO Peptides: Chemistry, Structure and Biology, Proceedings of the American Peptide Symposium, 14th, Columbus, Ohio, June 18-23, 1995 (1996), Meeting Date 1995, 851-852. Editor(s): Kaumaya, Pravin T. P.; Hodges, Robert S. Publisher: Mayflower Scientific, Kingswinford, UK.
CODEN: 63NTAF
DT Conference
LA English
AB Platelet aggregation is essential in the maintenance of hemostasis, but its malfunction may cause serious cardiovascular and cerebrovascular diseases. Inhibition of such pathol. platelet aggregation has been an attractive target for drug design efforts, which have mainly focused on mimicking the RGD recognition sequence in fibrinogen , whose interaction with the platelet surface receptor, GPIIb/IIIa, is the essential final step in platelet aggregation cascade. We have rationally designed highly potent small mol. antagonists of GPIIb/IIIa conforming to a three-point pharmacophoric binding model shown below from our double-strand RGD peptide lead. This report discusses salient features of the SAR of these inhibitors.
IT **171505-85-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(new RGD peptide mimetics as efficient inhibitors of platelet aggregation)
RN 171505-85-4 CAPLUS
CN Glycine, N-[4-[(aminoiminomethyl)amino]benzoyl]-.beta.-alanyl-L-.alpha.-aspartyl-2-phenyl-, (2S)- (9CI) (CA INDEX NAME)

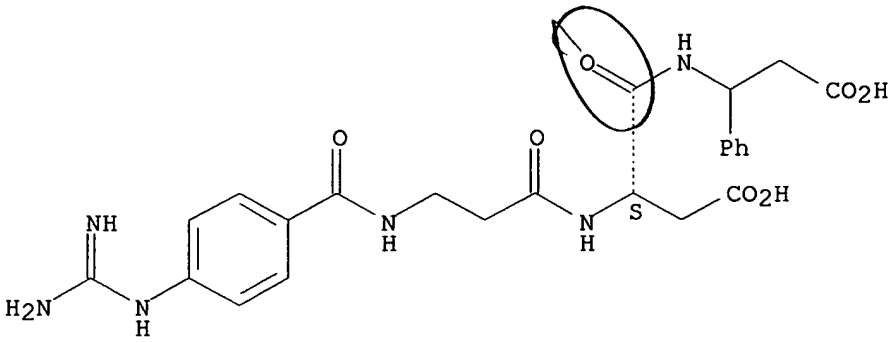
Absolute stereochemistry.



IT **171505-84-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(synthetic; new RGD peptide mimetics as efficient inhibitors of platelet aggregation)
RN 171505-84-3 CAPLUS
CN .beta.-Alanine, N-[4-[(aminoiminomethyl)amino]benzoyl]-.beta.-alanyl-L-

.alpha.-aspartyl-3-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

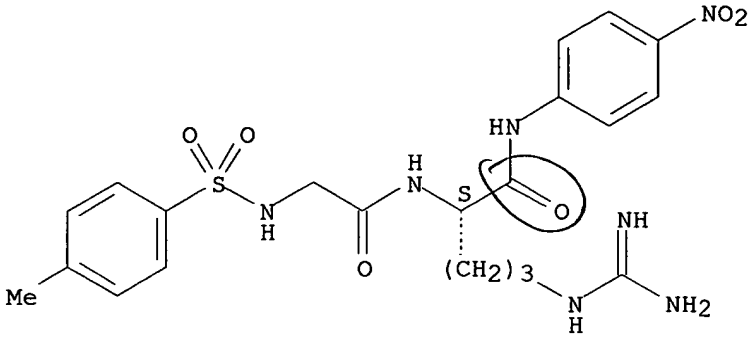


L27 ANSWER 25 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1996:560491 CAPLUS
DN 125:215690
TI Methods of determining endogenous thrombin potential and thrombin substrates for use in said methods
IN Hemker, Hendrik Coenraad; Rijkers, Dirk Thomas Sigurd; Tesser, Godefriedus Ignatius
PA Neth.
SO PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9621740	A1	19960718	WO 1996-NL18	19960110
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN				
	AU 9646348	A1	19960731	AU 1996-46348	19960110
	EP 802986	A1	19971029	EP 1996-902007	19960110
	EP 802986	B1	20010919		
	R: CH, DE, ES, FR, GB, IT, LI, NL				
	ES 2162025	T3	20011216	ES 1996-902007	19960110
	US 6207399	B1	20010327	US 1997-860808	19970905
PRAI	EP 1995-200043	A	19950110		
	WO 1996-NL18	W	19960110		

OS MARPAT 125:215690
AB A method for detg. the ETP (endogenous thrombin potential) of a sample, preferably in a continuous assay is claimed, said sample comprising a total anticoagulant activity of or equiv. to at least 0,07 U ISH/mL, wherein a thrombin substrate or a salt thereof that is sol. in the sample is applied in a manner known per se for detg. the ETP of a sample, said thrombin substrate being selected from the group comprising substrates of the formula P-Val-Xaa-S (P = nonarom., polar amino protective group; Val = valine residue attached via a peptide bond to Xaa; Xaa = amino acid residue comprising a terminal guanidino group or ureido group sepd. by at least 2 carbon atoms from the peptide backbone, said amino acid residue being attached to S; S = signal group such as a chromophore that can be enzymically hydrolyzed). Other substrates such as Zaa-Pipecolyl-Yaa-S or Zaa-Pro-Yaa-S, (Zaa = D-Phe, D-Trp, D-Tyr; Pro = proline; Yaa = amino acid residue other than Arg; S = signal group) can also be used. The substrates Boc-Gly-Val-Arg-pNA and H-Glu-Gly-Val-Arg-pNA are also applicable. Furthermore ETP detn. methods as such can be improved by addn. of hydroxylamine to the sample to circumvent defibrination of the sample.
IT **167961-67-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methods of detg. endogenous thrombin potential and thrombin substrates for use in said methods)
RN 167961-67-3 CAPLUS
CN L-Argininamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



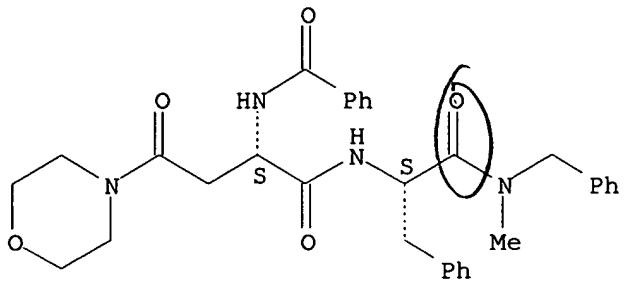
● HCl

L27 ANSWER 26 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1996:494173 CAPLUS
DN 125:143330
TI Peptide compounds for prevention and/or treatment of nitric oxide (NO)-mediated diseases
IN Itoh, Yoshikuni; Iwamoto, Toshiro; Yatabe, Takumi; Hamashima, Hitoshi; Inoue, Takayuki; Hashimoto, Seiji; Oku, Teruo
PA Fujisawa Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 739 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9616981	A2	19960606	WO 1995-JP2428	19951129
	WO 9616981	A3	19960906		
	W: AU, CA, CN, FI, HU, JP, KR, MX, NO, NZ, RU, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9539937	A1	19960619	AU 1995-39937	19951129
	EP 796270	A2	19970924	EP 1995-938602	19951129
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
	ZA 9510201	A	19960625	ZA 1995-10201	19951130
	US 5932737	A	19990803	US 1997-849076	19970530
PRAI	GB 1994-24408	A	19941202		
	GB 1995-4891	A	19950310		
	GB 1995-10042	A	19950518		
	WO 1995-JP2428	W	19951129		

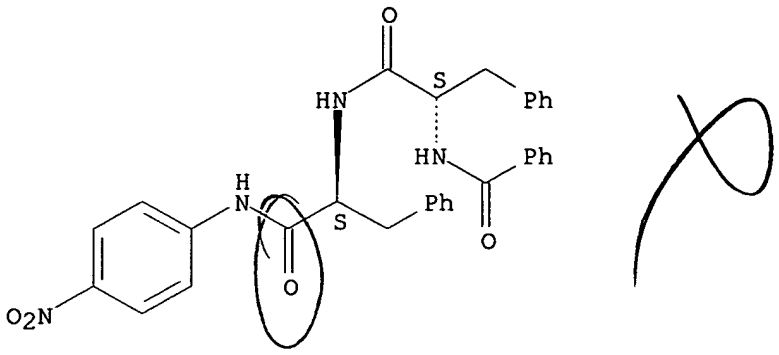
OS MARPAT 125:143330
AB Peptides WA1NR8CH(A2T)CONR9CH(A3R3)R4 [W = alkyl, (un)substituted aryl or fluorenyl, etc.; A1 = alkylene, NHCO, CO, CS, SO2; A2 = alkylene; T = H, aryl, heterocyclyl, OH, etc.; R8 = H, alkyl; R8 may link with A2T to form CH2C6H4CH2-o (Q); A3 = bond, alkylene; R3 = H, aryl, OH, etc.; R9 = H, alkyl or may link with A3R3 to form Q; R4 = CO2H, protected carboxy, carboxamido, etc. or CH(A3R3)R4 = N-alkyl-2-oxoquinoline moiety] or their pharmaceutically acceptable salts were prepd. for use as medicaments. Thus, dipeptide I was prepd. by acylation of aspartylphenylalaninamide deriv. with 2-benzofurancarboxylic acid. I and six other peptides showed 100% inhibition of NO prodn. in tests of murine macrophage cells.
IT **179879-70-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptides for prevention and/or treatment of nitric oxide-mediated diseases)
RN 179879-70-0 CAPLUS
CN L-Phenylalaninamide, N-benzoyl-4-(4-morpholinyl)-4-oxo-L-2-aminobutanoyl-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 27 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1996:347926 CAPLUS
DN 125:105712
TI Pharmacological characterization of novel tissue kallikrein inhibitors in vivo
AU Bizeto, Luciana; Antunes, Edson; Portaro, Fernanda C. V.; Juliano, Maria Aparecida; Juliano, Luiz; Prado, Eline S.; Nucci, Gilberto de
CS Departments of Pharmacology, Faculty of Medical Sciences, UNICAMP, PO Box 6111, 13081-970-Campinas-SP, Brazil
SO Immunopharmacology (1996), 32(1-3), 111-114
CODEN: IMMUDP; ISSN: 0162-3109
PB Elsevier
DT Journal
LA English
AB In this study we have investigated the effect of novel tissue kallikreins on the plasma protein exudation induced by porcine pancreatic kallikrein (PPK) in the rabbit skin in vivo. The tissue kallikrein inhibitors here described were synthesized based on analogs of peptide substrates for tissue kallikreins. The intradermal injection of PPK and rabbit urinary kallikrein, but not of rabbit plasma kallikrein, significantly increased the microvascular permeability leading to local edema formation in the rabbit skin. At the dose of 3-200 nmol/site, the intradermal co-administration of the tissue kallikrein inhibitors Bz-F-F-S-R-EDDnp (Ki = 0.1 .mu.M; ESP5), PAC-F-S-R-EDDnp (Ki = 0.7 .mu.M; ESP6), Bz-F-F-A-P-R-NH2 (Ki = 7.8 .mu.M; ESP8), PAC-F-F-R-P-R-NH2 (Ki = 0.3 .mu.M; ESP9) and Bz-F-F-S-R-NH2 (Ki = 0.3 .mu.M; ESP11) dose-dependently inhibited the plasma protein exudation induced by PPK. The most potent compd. was ESP6 (IC25 = 7.8 nmol/site) followed by ESP5 (IC25 = 14.2 nmol/site), ESP8 (IC25 = 25 nmol/site), ESP9 (IC25 = 30 nmol/site) and ESP11 (IC25 = 50.4 nmol/site). The compds. Bz-F-F-R-P-R-NH2 (Ki = 0.5 .mu.M; ESP1), Bz-F-F-pNa (Ki = 0.4 .mu.M; ESP3), Bz-F(NH2)-F-R-P-R-NH2 (Ki = 1.1 .mu.M; ESP7) and Bz-F-F-S-P-R-NH2 (Ki = 4.6 .mu.M; ESP10) had no significant effect on the PPK-induced plasma protein exudation in doses up to 200 nmol/site. ESP6 also inhibited the PPK-induced plasma protein exudation when administered systemically. This compd. may constitute a useful tool to further investigate both the physiol. and pathol. role of tissue kallikreins.
IT **179166-91-7**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(effect on skin plasma protein exudation induced by kallikrein)
RN 179166-91-7 CAPLUS
CN L-Phenylalaninamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


O
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HN
Ph
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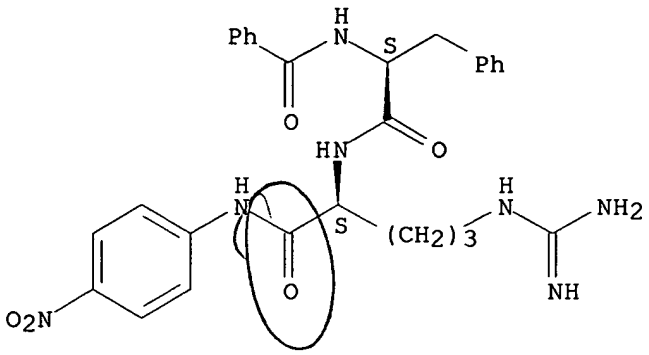
S
Ph
O
O
O2N

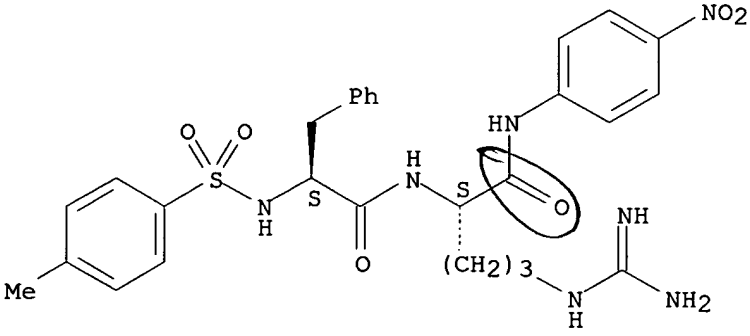
L27 ANSWER 28 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1996:249130 CAPLUS
DN 124:282965
TI Kinetic characterization of rat tissue kallikrein using N.alpha.-substituted arginine 4-nitroanilides and N.alpha.-benzoyl-L-arginine ethyl ester as substrates
AU Sousa, M.O.; Rodrigues, C.V.; Pena, H.B.; Alvarenga, M.G.; Machado-Coelho, G.L.L.; Santoro, M.M.; Juliano, M.A.; Juliano, L.; Figueiredo, A.F.S.
CS Faculdade de Farmacia, Universidade Federal de Minas Gerais, Belo Horizonte, 30150-112, Brazil
SO Brazilian Journal of Medical and Biological Research (1996), 29(3), 327-34
CODEN: BJMRDK; ISSN: 0100-879X
PB Associacao Brasileira de Divulgacao Cientifica
DT Journal
LA English
AB Hydrolysis of seven N.alpha.-substituted L-arginine 4-nitroanilides: benzoyl-arginine p-nitroanilide (Bz-Arg-Nan), tosyl-arginine p-nitroanilide (Tos-Arg-Nan), acetyl-leucyl-arginine p-nitroanilide (Ac-Leu-Arg-Nan), acetyl-phenylalanyl-arginine p-nitroanilide (Ac-Phe-Arg-Nan), benzoyl-phenylalanyl-arginine p-nitroanilide (Bz-Phe-Arg-Nan), tosyl-phenylalanyl-arginine p-nitroanilide (Tos-Phe-Arg-Nan), and D-valyl-leucyl-arginine p-nitroanilide (D-Val-Leu-Arg-Nan), and the N.alpha.-substituted L-arginine ester: benzoyl-arginine Et ester (Bz-Arg-OEt), by rat tissue kallikrein was studied throughout a wide range of substrate concns. The enzyme showed a bimodal behavior with all the substrates tested except Tos-Arg-Nan. At low substrate concns. (10 to 170 .mu.M for p-nitroanilides and 50 to 190 .mu.M for Bz-Arg-OEt), the hydrolysis followed Michaelis-Menten kinetics, but at higher substrate concns. (150 to 700 .mu.M for p-nitroanilides and 200 to 1800 .mu.M for Bz-Arg-OEt), a deviation from Michaelis-Menten kinetics was obsd. with a significant decrease in hydrolysis rates. At high concns. of the p-nitroanilide substrates, partial enzyme inhibition was obsd., whereas complete enzyme inhibition was obsd. with Bz-Arg-OEt at high concn. The kinetic parameters reported here were calcd. from data for substrate concn. ranges where the enzyme followed Michaelis-Menten behavior. D-Val-Leu-Arg-Nan (Km = 24 .+-. 2 .mu.M; Vmax = 10.42 .+-. 0.28 .mu.M/min) was the best substrate tested, followed by Ac-Phe-Arg-Nan (Km = 13 .+-. 2 .mu.M; Vmax = 3.21 .+-. 0.11 .mu.M/min), while Tos-Arg-Nan (Km = 29 .+-. 2 .mu.M; Vmax = 0.10 .+-. 0.002 .mu.M/min) was the worst of the tested substrates for rat tissue kallikrein. For the hydrolysis of Bz-Arg-OEt (Km = 125 .+-. 15 .mu.M; Vmax = 121.3 .+-. 7.6 .mu.M/min), the kinetic parameters using a substrate inhibition model can reasonably account for the obsd. enzyme behavior, with a Ksi value about 13.6 times larger than the estd. Km value.
IT **103418-68-4 175888-94-5**, Tosyl-phenylalanyl-arginine p-nitroanilide
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(as kallikrein substrate; kinetic characterization of rat submandibular gland kallikrein using N.alpha.-substituted arginine 4-nitroanilides and N.alpha.-benzoyl-L-arginine Et ester as substrates)
RN 103418-68-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



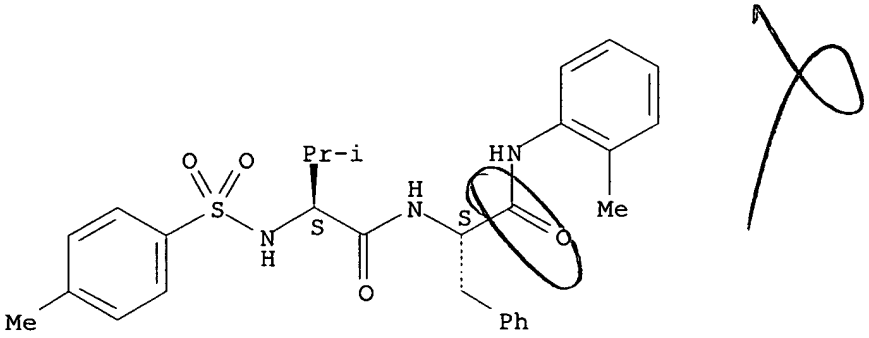
RN 175888-94-5 CAPLUS
CN L-Argininamide, N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



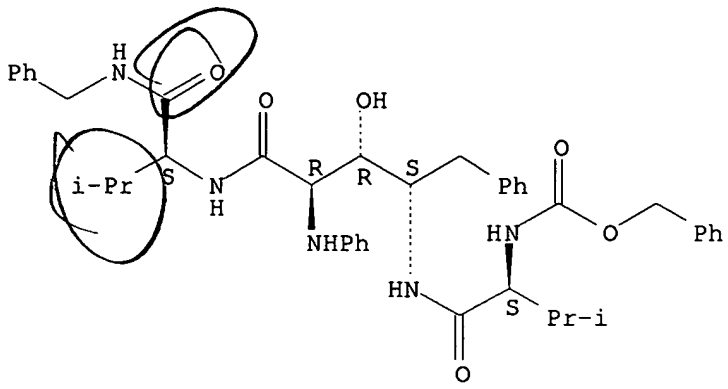
L27 ANSWER 29 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1996:235940 CAPLUS
DN 125:11404
TI Synthesis of some new sulfonamides derivatives of toluidine as possible antimicrobial agents
AU Abbas, Y. A.
CS Faculty Education, Tanta University, Kafr El-Sheikh, Egypt
SO Egyptian Journal of Pharmaceutical Sciences (1995), 36(1-6), 187-95
CODEN: EJPSBZ; ISSN: 0301-5068
PB National Information and Documentation Centre
DT Journal
LA English
AB The synthesis of amino acid amides was reported. Example compds. are the amino acid amides I (R = Me, Ph, etc.) or II (same R) and dipeptide analogs. Some compds. were screened for antimicrobial, bactericidal and fungicidal activity.
IT **177267-28-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and biocidal activity of amino acid amide derivs.)
RN 177267-28-6 CAPLUS
CN L-Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]-L-valyl-N-(2-methylphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



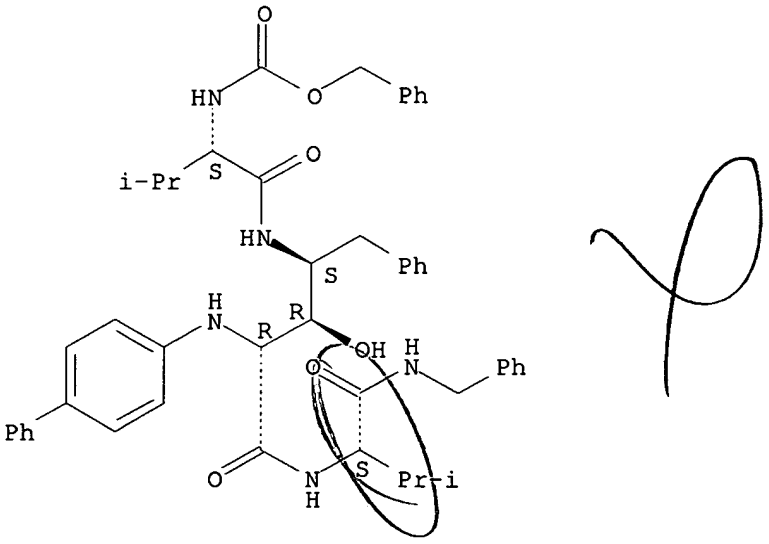
L27 ANSWER 30 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1995:938729 CAPLUS
DN 124:105558
TI 3D-Quantitative Structure-Activity Relationships of Human Immunodeficiency Virus Type-1 Proteinase Inhibitors: Comparative Molecular Field Analysis of 2-Heterosubstituted Statine Derivatives-Implications for the Design of Novel Inhibitors
AU Kroemer, Romano T.; Ettmayer, Peter; Hecht, Peter
CS SANDOZ Forschungsinstitut Ges. m. b. H, Vienna, A-1235, Austria
SO Journal of Medicinal Chemistry (1995), 38(25), 4917-28
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB A set of 100 novel 2-heterosubstituted statine derivs. inhibiting human immunodeficiency virus type-1 proteinase has been investigated by comparative mol. field anal. To combine the structural information available from x-ray analyses with a predictive quant. structure-activity relation (QSAR) model, docking expts. of a prototype compd. into the receptor were performed, and the 'active conformation' was detd. The structure of the receptor was taken from the published x-ray anal. of the proteinase with bound MVT-101, the latter compd. exhibiting high structural similarity with the inhibitors investigated. The validity of the resulting QSARs was confirmed in four different ways. (1) The common parameters, namely, the cross-validated r2 values obtained by the leave-one-out (LOO) method (r2ev = 0.572-0.593), and (2) the accurate prediction of a test set of 67 compds. (q2 = 0.552-0.569) indicated a high consistency of the models. (3) Repeated analyses with two randomly selected cross-validation groups were performed and the cross-validated r2 values monitored. The resulting av. r2 values were of similar magnitudes compared to those obtained by the LOO method. (4) The coeff. fields were compared with the steric and electrostatic properties of the receptor and showed a high level of compatibility. Further anal. of the results led to the design of a novel class of highly active compds. contg. an addnl. linkage between P1' and P3'. The predicted activities of these inhibitors were also in good agreement with the exptl. detd. values.
IT **161510-37-8**, SDZ 282329 **161510-42-5**, SDZ 282700
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3D-quant. structure-activity relationships of human immunodeficiency virus type-1 proteinase inhibitors using comparative mol. field anal. of 2-heterosubstituted statine derivs.)
RN 161510-37-8 CAPLUS
CN L-Lyxonamide, 2,4,5-trideoxy-4-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-N-[2-methyl-1-[[(phenylmethyl)amino]carbonyl]propyl]-5-phenyl-2-(phenylamino)-, [1(S),4(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 161510-42-5 CAPLUS
CN L-Lyxonamide, 2-([1,1'-biphenyl]-4-ylamino)-2,4,5-trideoxy-4-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-N-[2-methyl-1-[[(phenylmethyl)amino]carbonyl]propyl]-5-phenyl-, [1(S),4(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 31 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1995:820544 CAPLUS
DN 123:227821
TI Preparation of 4-amidinophenylsulfonamide antithrombotics
IN Leinert, Herbert; Poll, Thomas; von der Saal, Wolfgang; Stegmeier, Karlheinz
PA Boehringer Mannheim G.m.b.H., Germany
SO Ger. Offen., 10 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

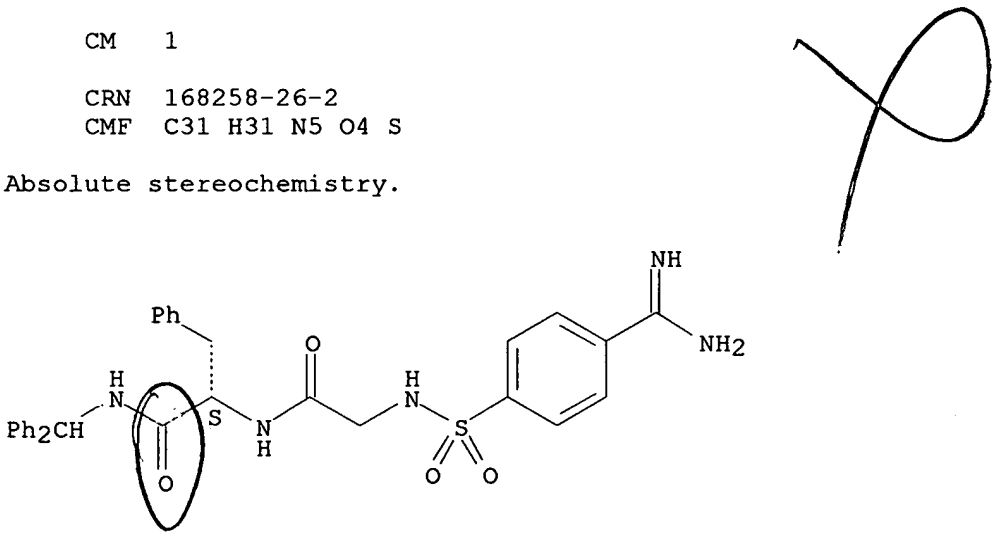
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4316922	A1	19941124	DE 1993-4316922	19930520
	WO 9427958	A1	19941208	WO 1994-EP1562	19940513
	W: AU, BG, BR, CA, CN, CZ, FI, HU, JP, KR, KZ, NO, NZ, PL, RO, RU, SI, SK, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9469278	A1	19941220	AU 1994-69278	19940513
PRAI	DE 1993-4316922		19930520		
	WO 1994-EP1562		19940513		

OS MARPAT 123:227821
AB The title compds. (I; A = .alpha.-amino acid residue; B = H, A; R1, R2 = H, Ph, CO2H, alkoxycarbonyl), useful as agents for treating thromboembolic diseases (no data), are prepd.
IT **168258-27-3P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 4-amidinophenylsulfonamide antithrombotics)
RN 168258-27-3 CAPLUS
CN L-Phenylalaninamide, N-[[4-(aminoiminomethyl)phenyl]sulfonyl]glycyl-N-(diphenylmethyl)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

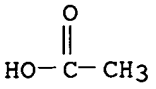
CRN 168258-26-2
CMF C31 H31 N5 O4 S

Absolute stereochemistry.



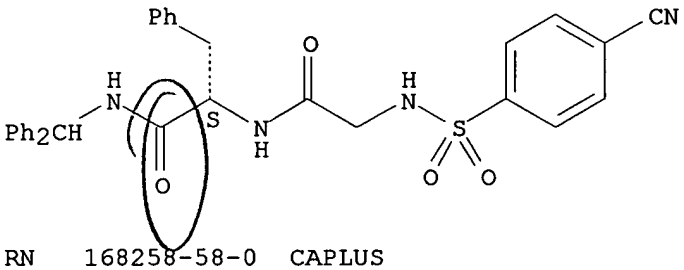
CM 2

CRN 64-19-7
CMF C2 H4 O2



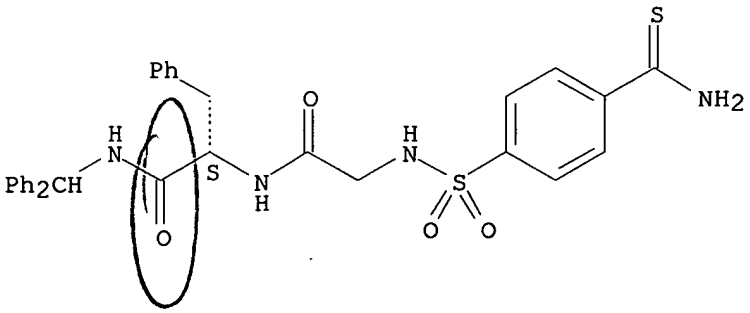
IT **168258-57-9P 168258-58-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of 4-amidinophenylsulfonamide antithrombotics from)
RN 168258-57-9 CAPLUS
CN L-Phenylalaninamide, N-[(4-cyanophenyl)sulfonyl]glycyl-N-(diphenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 168258-58-0 CAPLUS
CN L-Phenylalaninamide, N-[[4-(aminothioxomethyl)phenyl]sulfonyl]glycyl-N-(diphenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

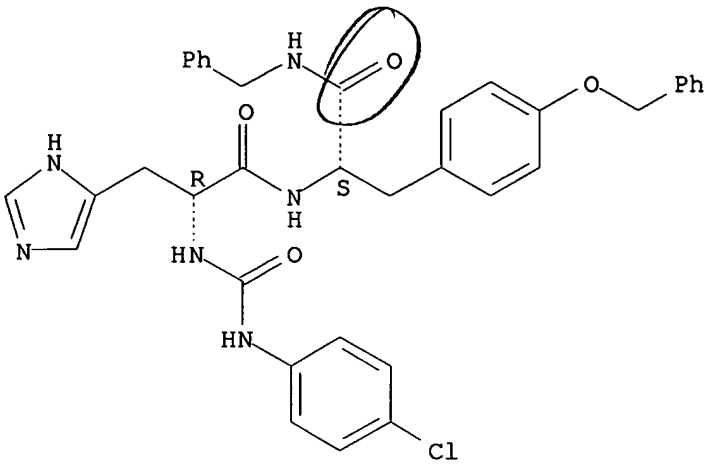


L27 ANSWER 32 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1995:812991 CAPLUS
DN 123:228919
TI Preparation of substituted di- and tripeptide inhibitors of protein:farnesyl transferase
IN Bolton, Gary Louis; Creswell, Mark Wallace; Hodges, John Cooke; Wilson, Michael William
PA Warner Lambert Co., USA
SO PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9512612	A1	19950511	WO 1994-US11553	19941012
	W: AM, AU, BG, BY, CA, CZ, EE, FI, GE, HU, JP, KG, KR, NO, NZ, PL, RO, RU, SI, UA				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2170766	AA	19950511	CA 1994-2170766	19941012
	AU 9479760	A1	19950523	AU 1994-79760	19941012
	AU 681454	B2	19970828		
	EP 730605	A1	19960911	EP 1994-930725	19941012
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09504547	T2	19970506	JP 1995-513224	19941012
	HU 75308	A2	19970528	HU 1996-1193	19941012
	FI 9601819	A	19960429	FI 1996-1819	19960429
	NO 9601814	A	19960506	NO 1996-1814	19960503
	US 5830868	A	19981103	US 1996-671460	19960627
PRAI	US 1993-148735	A	19931105		
	US 1994-303301	A	19940913		
	WO 1994-US11553	W	19941012		

OS MARPAT 123:228919
AB Novel protein:farnesyl transferase enzyme inhibitors I [n = 1, 2; A = COR3, CO2R3, CONHR3, CSR3, C(S)OR3, CSNHR3, CF3SO2, aryl-SO2, alkyl-SO2; R3 = alkyl, (CH2)m-cycloalkyl, (CH2)m-aryl, (CH2)m-heteroaryl, (CH2)mO-alkyl; m = 0-3; R, Y, Z = independently H, Me; R1 = H, CO-aryl, (CH2)m-aryl, O(CH2)m-cycloalkyl, O(CH2)m-aryl, O(CH2)m-heteroaryl, (CH2)mO-alkyl, located at the meta or para position; X = 1-4 substituents H, alkyl, CF3, F, Cl, Br, iodo, HO, MeO, NO2, NH2, NMe2, OPO3H2, CH2PO3H2; R2 = NR(CH2)nCO2R3, NR(CH2)nCONHR3, NR(CH2)nR3, NR(CH2)nCH2OR4, NR(CH2)nCH2SR4, NRCH(COR5)(CH2)n-heteroaryl, NRCH(COR5)(CH2)nOR3, NRCH(COR5)(CH2)nSR3, etc.; R4 = H, R3; R5 = OH, NH2, OR3, NHR3], optical isomers, diastereomers, or pharmaceutically acceptable salts thereof are claimed and described, as well as methods for prepn. and pharmaceutical compns., which are useful in controlling tissue proliferative diseases, including cancer and restenosis. Thus, PhCH2O2C-D-His-L-Tyr(CH2Ph)-L-Ser(CH2Ph)-NHEt, prepd. via std. soln. peptide coupling reactions, inhibited protein:farnesyl transferase with IC50 = 0.028 .mu.M.
IT **168174-53-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of substituted di- and tripeptide inhibitors of protein:farnesyl transferase)
RN 168174-53-6 CAPLUS
CN L-Tyrosinamide, N-[[(4-chlorophenyl)amino]carbonyl]-D-histidyl-N,O-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


Ph
H
N
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O
Ph
H
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R
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H
S
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HN
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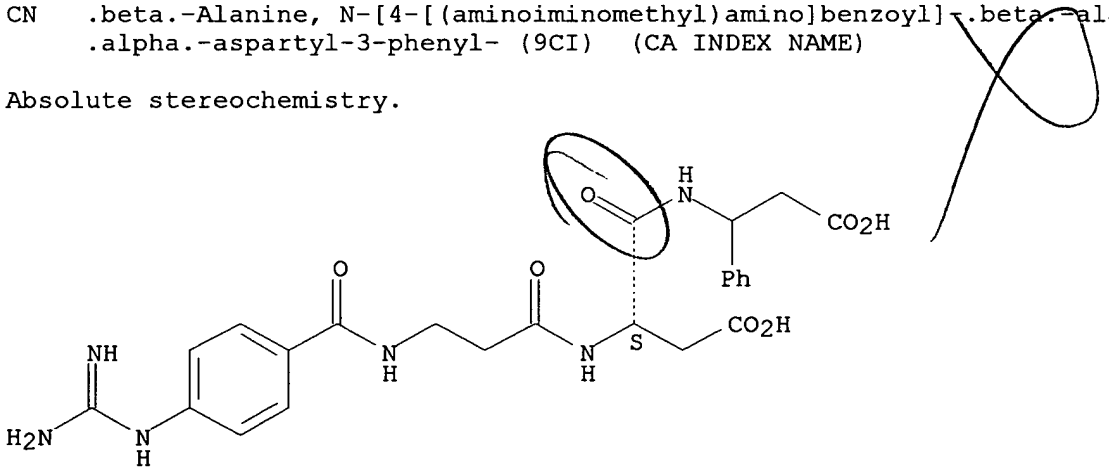
HN
Cl

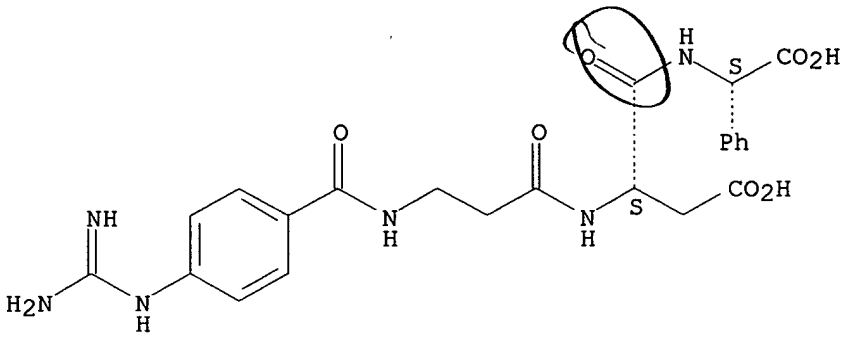
L27 ANSWER 33 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1995:796289 CAPLUS
DN 124:30348
TI Design, synthesis and SAR of RGD peptide hybrids as highly efficient inhibitors of platelet aggregation
AU Ojima, Iwao; Dong, Qing; Chakravarty, Subrata; Peerschke, Ellinor; Hwang, Shing Mei; Wong, Angela S.
CS School of Medicine, State University of New York at Stony Brook, Stony Brook, NY, 11794, USA
SO Bioorganic & Medicinal Chemistry Letters (1995), 5(17), 1941-6
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier
DT Journal
LA English
AB A new series of peptide hybrids is developed as highly potent and selective antagonists of the GPIIb/IIIa receptor through rational modification of the RGDX sequence. Structure-activity relationships of these peptide hybrids have disclosed the important role of the C-terminal hydrophobic moiety and the N-terminal arginine side chain surrogates. Mol. modeling study strongly suggests the significance of a .gamma.-turn conformation to achieve exceedingly high activity and receptor specificity.
IT **171505-84-3P 171505-85-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(design, synthesis and structure activity relationship of RGD peptide hybrids as highly efficient inhibitors of platelet aggregation)
RN 171505-84-3 CAPLUS
CN .beta.-Alanine, N-[4-[(aminoiminomethyl)amino]benzoyl]-.beta.-alanyl-L-.alpha.-aspartyl-3-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



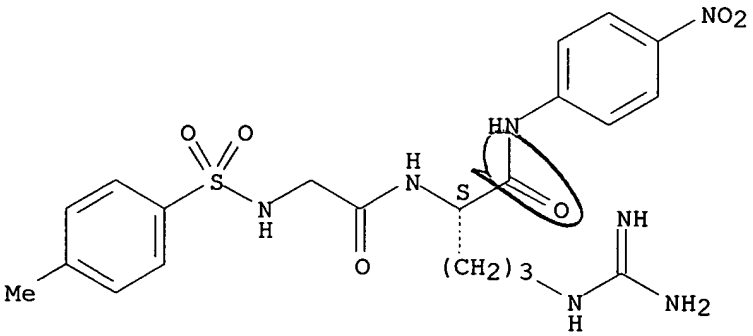
RN 171505-85-4 CAPLUS
CN Glycine, N-[4-[(aminoiminomethyl)amino]benzoyl]-.beta.-alanyl-L-.alpha.-aspartyl-2-phenyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 34 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1995:762217 CAPLUS
DN 123:192056
TI Design and synthesis of thrombin substrates with modified kinetic parameters
AU Rijkers, Dirk T. S.; Welders, Simone J. H.; Tesser, Godefridus I.; Hemker, H. Coenraad
CS Faculty of Medicine, University of Limburg, Maastricht, 6200 MD, Neth.
SO Thrombosis Research (1995), 79(5/6), 491-9
CODEN: THBRAA; ISSN: 0049-3848
PB Elsevier
DT Journal
LA English
AB For the continuous registration of thrombin formation in plasma, selective thrombin substrates are required, that show moderate binding affinities (high Km) and low turnover nos. (low kcat). Previously the authors have used SQ68 (CH3O-CO-CH2-CO-Aib-Arg-pNA) for this purpose. To find more substrates suitable for this application, the authors synthesized a series of 25 peptide p-nitroanilides. As lead structures SQ68 and S2238 (H-D-Phe-Pip-Arg-pNA) were used. By introduction of specific structure modifications the authors tried to alter the kinetic data in the required direction. The modifications were designed on basis of existing knowledge on the structure of the thrombin active-site and its surroundings. The authors indeed obtained a no. of substrates with the kinetic consts. in the desired range.
IT **167961-67-3P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(design and synthesis of peptide p-nitroanilides and reaction with human .alpha.-thrombin and factor Xa)
RN 167961-67-3 CAPLUS
CN L-Argininamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

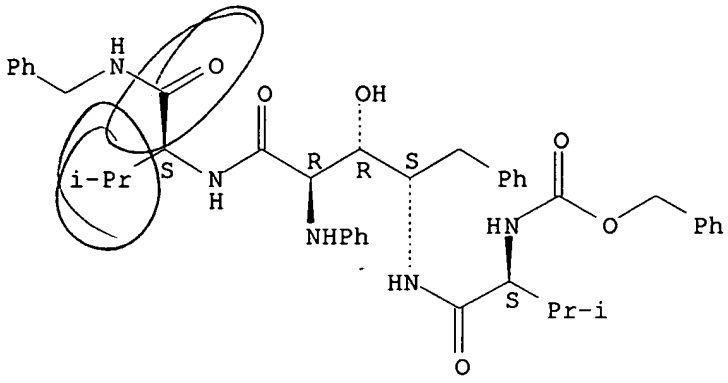
Absolute stereochemistry.



● HCl

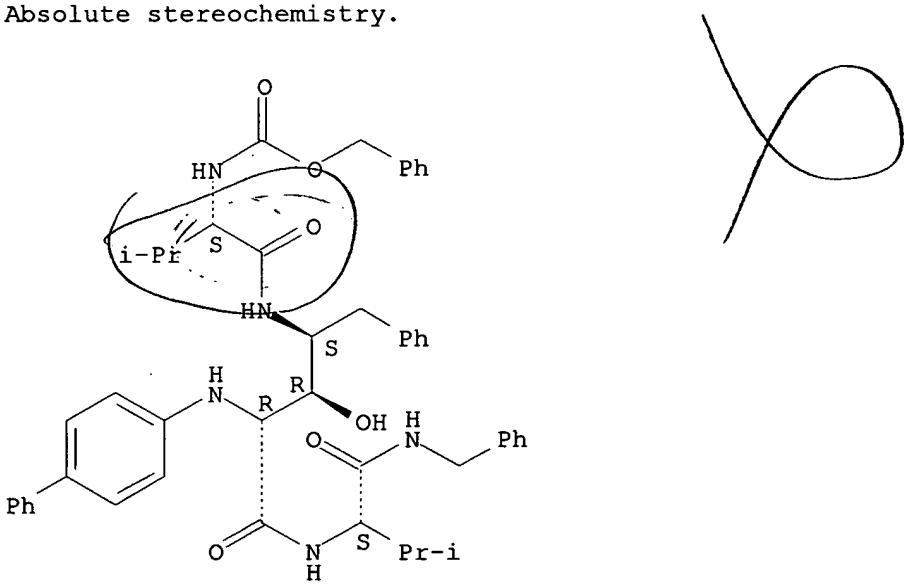
L27 ANSWER 35 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1995:43426 CAPLUS
DN 122:188109
TI Inhibitors of HIV-1 Proteinase Containing 2-Heterosubstituted 4-Amino-3-hydroxy-5-phenylpentanoic Acid: Synthesis, Enzyme Inhibition, and Antiviral Activity
AU Scholz, Dieter; Billich, Andreas; Charpiot, Brigitte; Ettmayer, Peter; Lehr, Philipp; Rosenwirth, Brigitte; Schreiner, Erwin; Gstach, Hubert
CS Department of Antiretroviral Therapy, SANDOZ Forschungsinstitut Ges.m.b.H., Vienna Austria, A-1235, Austria
SO Journal of Medicinal Chemistry (1994), 37(19), 3079-89
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB A convenient procedure for the synthesis of 2-hetero-substituted statine derivs. as novel building blocks in HIV-protease inhibitors has been developed. The synthesis starts with protected L-phenylalaninols, which were converted to .gamma.-amino .alpha.,.beta.-unsatd. esters in a one-pot procedure. A highly diastereoselective epoxidn. of the N-protected (E)-enoates, followed by regioselective ring opening of the corresponding 2,3-epoxy esters with a variety of heteronucleophiles, resulted in 2-hetero-substituted statine derivs., e.g. I [R = CH2Ph, Ph, CH2CH2Ph, Bu, cyclohexyl, 1-naphthyl, 4-PhC6H4 2-(3-indolyl)ethyl, 2-(2-pyridyl)ethyl, CH2C6H4OMe-4, CH2C6H4Cl-4, CH2C6H4Br-4; X = Val, Ala, Leu, Ile, L-tert-leucine (L-Tle), D-Tle, L-2-aminobutanoic acid, Trp, L-phenylglycine, Asn, Ser, Glu, His' X1 = Val, Leu, Ile, L-Tle, D-Tle, Asn]. The overall stereochem. outcome of the transformations meets the required configuration of HIV-protease inhibitors. The short, synthetically flexible, and highly diastereoselective synthesis of 2-heterosubstituted statines has enabled a broad derivation covering the S3, S2, and S1'-S3' sites of the enzyme. In a series of 46 derivs., several potent inhibitors were obtained with Ki values as low as 3.4 nM and antiviral activity in the lower nanomolar-range. The structural parameters of the compds. which det. the potency of inhibition and selectivity for the viral enzyme are discussed.
IT **161510-37-8P 161510-42-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn., HIV proteinase inhibition, and antiviral activity of hetero-substituted amino(hydroxy)phenylpentanoic acids)
RN 161510-37-8 CAPLUS
CN L-Lyxonamide, 2,4,5-trideoxy-4-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-N-[2-methyl-1-[[(phenylmethyl)amino]carbonyl]propyl]-5-phenyl-2-(phenylamino)-, [1(S),4(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 161510-42-5 CAPLUS
CN L-Lyxonamide, 2-([1,1'-biphenyl]-4-ylamino)-2,4,5-trideoxy-4-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-N-[2-methyl-1-[[(phenylmethyl)amino]carbonyl]propyl]-5-phenyl-, [1(S),4(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 36 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1994:701334 CAPLUS
DN 121:301334
TI Preparation of ureidopeptides as inhibitors of thrombocyte aggregation, cancer cell metastasis, and osteoclast binding to bone surfaces.
IN Klingler, Otmar; Just, Melitta; Breipohl, Gerhard; Koenig, Wolfgang; Jablonka, Bernd; Zoller, Gerhard; Knolle, Jochen; Stilz, Hans Ulrich
PA Cassella AG, Germany
SO Ger. Offen., 16 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4309867	A1	19940929	DE 1993-4309867	19930326
	CA 2155843	AA	19941013	CA 1994-2155843	19940309
	WO 9422907	A1	19941013	WO 1994-EP713	19940309
	W: AU, CA, HU, JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9463754	A1	19941024	AU 1994-63754	19940309
	AU 679509	B2	19970703		
	EP 689549	A1	19960103	EP 1994-911129	19940309
	EP 689549	B1	19980617		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	HU 73409	A2	19960729	HU 1995-2792	19940309
	HU 219483	B	20010428		
	JP 08508267	T2	19960903	JP 1994-521591	19940309
	AT 167483	E	19980715	AT 1994-911129	19940309
	ES 2119187	T3	19981001	ES 1994-911129	19940309
	ZA 9402124	A	19941110	ZA 1994-2124	19940325
	IL 109135	A1	19990312	IL 1994-109135	19940325
	US 5703050	A	19971230	US 1996-513815	19960117
PRAI	DE 1993-4309867	A	19930326		
	WO 1994-EP713	W	19940309		

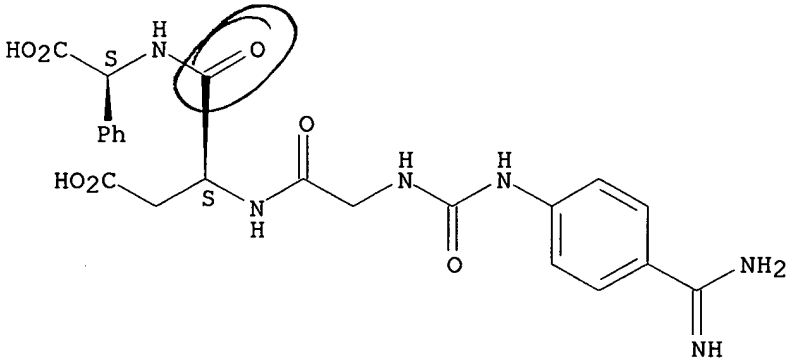
OS MARPAT 121:301334
AB R1AC(:Z)BNRCR2R3(CH2)rW [r = 0-3; Z = O, S; W = COW1, tetrazolyl, SO3H, SO2NHR9; W1 = OH, alkoxy, amino, (substituted) arylalkoxy, aryloxy; A = (CH2)kNRa, Q1; n, p = 0-4; k = 1-4; B = NRb(CH2)mCO, NRbCHRsCO, Q2, Q3; s, t = 0-5; Rs = amino acid side chain; Ra, Rb = H, OH, alkyl, hydroxycarbonylalkyl, alkoxycarbonylalkyl, (substituted) aryl, arylalkyl, aryloxy, arylalkoxy, etc.; R = H, alkyl; R1 = NHX, C(:NX)NH2; X = H,, cyano, OH, alkoxy, amino, alkyl, alkylcarbonyl, alkoxycarbonyl, (substituted) arylcarbonyl, aryloxycarbonyl, etc.; R2 = H, (substituted) alkyl, Ph; R3 = H, CO2R4, CONMeR4, CONHR4; R4 = H, (substituted) alkyl; R9 = H, aminocarbonyl, alkyl, cycloalkyl], were prepd. as inhibitors of thrombocyte aggregation, cancer cell metastasis, and osteoclast formation (no data). Thus, [3-[4-(aminoiminomethyl)phenyl]ureido]acetylaspartylphenylglycine was prepd. via coupling of [3-[4-(tert-butyloxycarbonylaminoiminomethyl)phenyl]ureido]acetic acid Na salt (prepd. in several steps starting from Et isocyanatoacetate and 4-aminobenzonitrile) with H-Asp(OtBu)-Phg-OtBu (Phg = phenylglycyl) using DCC, hydroxybenzotriazole, and ethylmorpholine in DMF at 0.degree..
IT **159216-52-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of ureidopeptides as inhibitors of thrombocyte aggregation,

cancer cell metastasis, and osteoclast binding to bone surfaces)

RN 159216-52-1 CAPLUS

CN Glycine, N-[N-[N-[[[4-(aminoiminomethyl)phenyl]amino]carbonyl]glycyl]-L-.alpha.-aspartyl]-L-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **159216-57-6P**

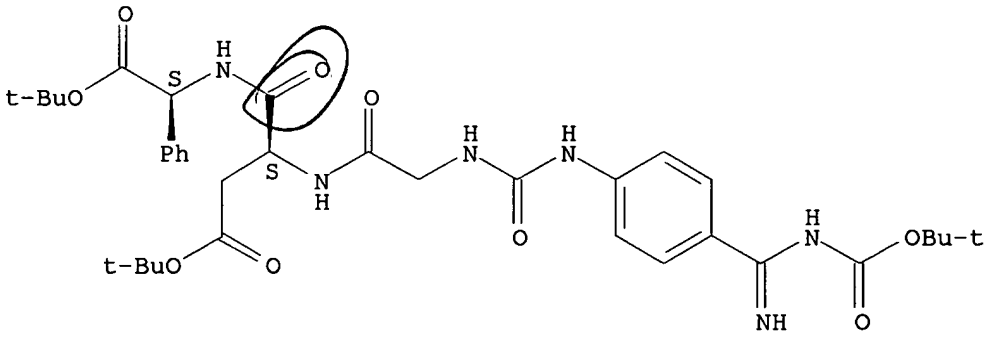
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of ureidopeptides as inhibitors of thrombocyte aggregation, cancer cell metastasis, and osteoclast binding to bone surfaces)

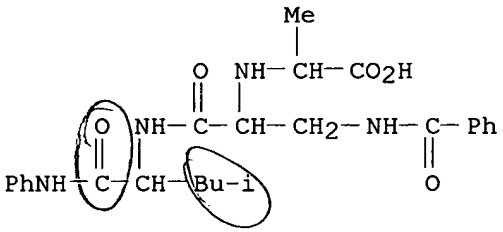
RN 159216-57-6 CAPLUS

CN Glycine, N-[N-[N-[[[4-[[[(1,1-dimethylethoxy)carbonyl]amino]iminomethyl]phenyl]amino]carbonyl]glycyl]-L-.alpha.-aspartyl]-L-2-phenyl-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

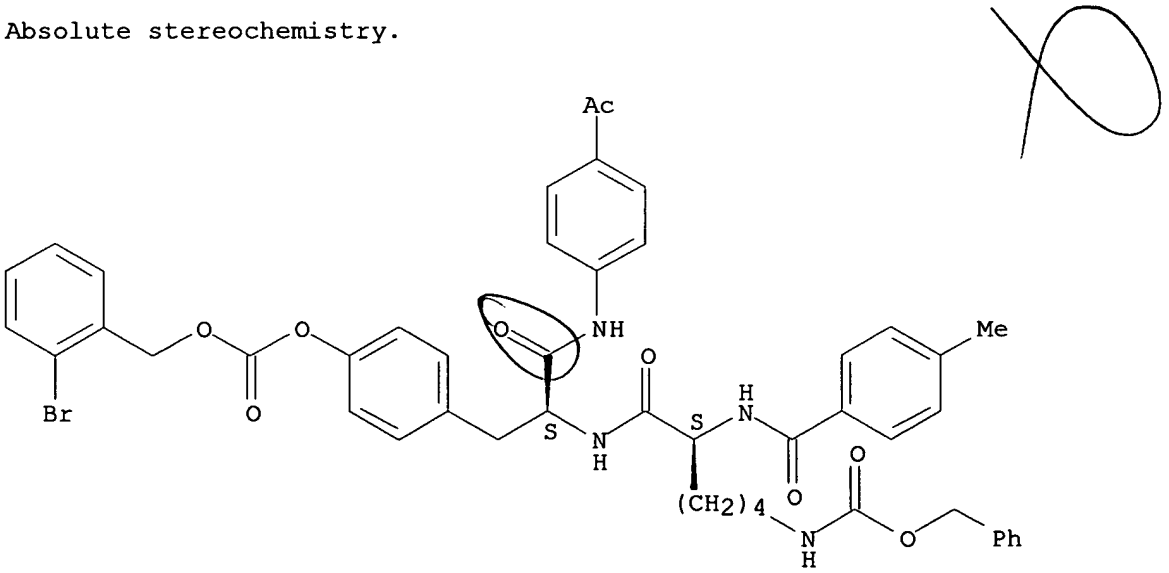


L27 ANSWER 37 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1994:271122 CAPLUS
DN 120:271122
TI Inhibition of matrix metalloproteinases by N-carboxyalkyl peptides
AU Chapman, Kevin T.; Kopka, Ihor E.; Durette, Philippe L.; Esser, Craig K.; Lanza, Thomas J.; Izquierdo-Martin, Maria; Niedzwiecki, Lisa; Chang, Benedict; Harrison, Richard K.; et al.
CS Dep. Med. Chem. Res., Merck Res. Lab., Rahway, NJ, 07065-0900, USA
SO Journal of Medicinal Chemistry (1993), 36(26), 4293-301
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB An extensive study of the requirements for effective binding of N-carboxyalkyl peptides to human stromelysin, collagenase, and to a lesser extent, gelatinase A has been investigated. These efforts afforded inhibitors generally in the 100-400 nM range for these matrix metalloproteinases. The most significant increase in potency was obtained with the introduction of a .beta.-phenylethyl group at the P1' position, suggesting a small hydrophobic channel into the S1' subsite of stromelysin. Compd. I is relatively selective for rabbit stromelysin with a Ki = 6.5 nM and may prove useful for elucidating the role of endogenously-produced stromelysin in lapine models of tissue degrdn.
IT **154652-06-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and inhibition by, of stromelysin, collagenase, and gelatinase A)
RN 154652-06-9 CAPLUS
CN L-Leucinamide, 3-(benzoylamino)-N-(1-carboxyethyl)-L-alanyl-N-phenyl-, (R)- (9CI) (CA INDEX NAME)



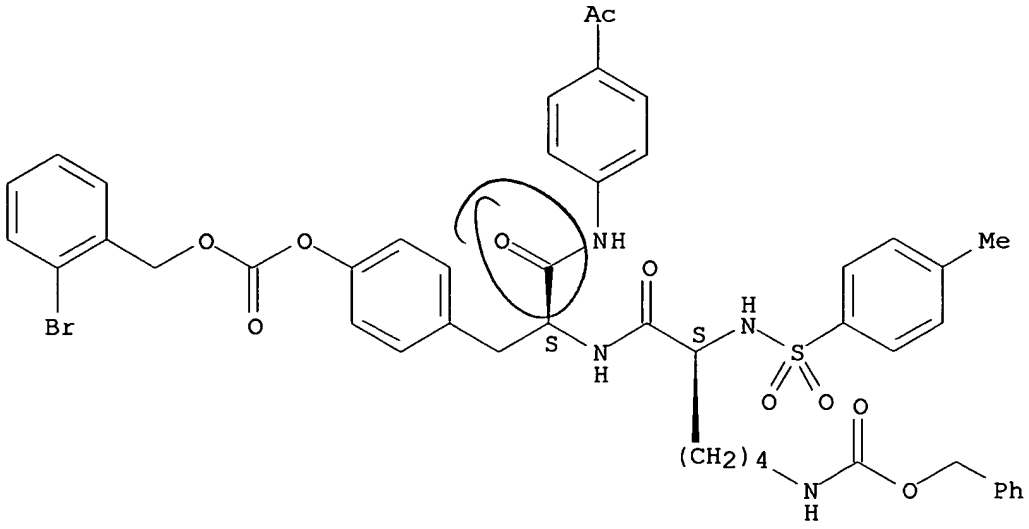
L27 ANSWER 38 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1994:135102 CAPLUS
DN 120:135102
TI Development of active center-directed plasmin and plasma kallikrein inhibitors and studies on the structure-inhibitory activity relationship
AU Teno, Naoki; Wanaka, Keiko; Okada, Yoshio; Taguchi, Hiroaki; Okamoto, Utako; Hijikata-Okunomiya, Akiko; Okamoto, Shosuke
CS Fac. Pharm. Sci., Kobe-Gekuin Univ., Kobe, 651-21, Japan
SO Chemical & Pharmaceutical Bulletin (1993), 41(6), 1079-80
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
AB Phenylalanine anilide I, a potent and selective inhibitor of plasma kallikrein, can be divided into three parts (P1, P1' and P2'), each of which contains one of the rings. Each part was substituted with various other moieties in order to study the relationship between the structure and inhibitory activities activities toward plasmin, plasma kallikrein, urokinase and thrombin. Tyrosine anilide II inhibited plasma and plasma kallikrein with IC50 values of 2.3 .times. 10-7 M and 3.7 .times. 10-7 M, and Ki values of 1.2 .times. 10-7M and 1.3 .times. 10-7, M., resp.
IT **120672-50-6P 152438-51-2P 152438-54-5P**
152438-55-6P 152438-56-7P 152438-57-8P
152519-60-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acidic deblocking of)
RN 120672-50-6 CAPLUS
CN L-Tyrosinamide, N2-(4-methylbenzoyl)-N6-[(phenylmethoxy)carbonyl]-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



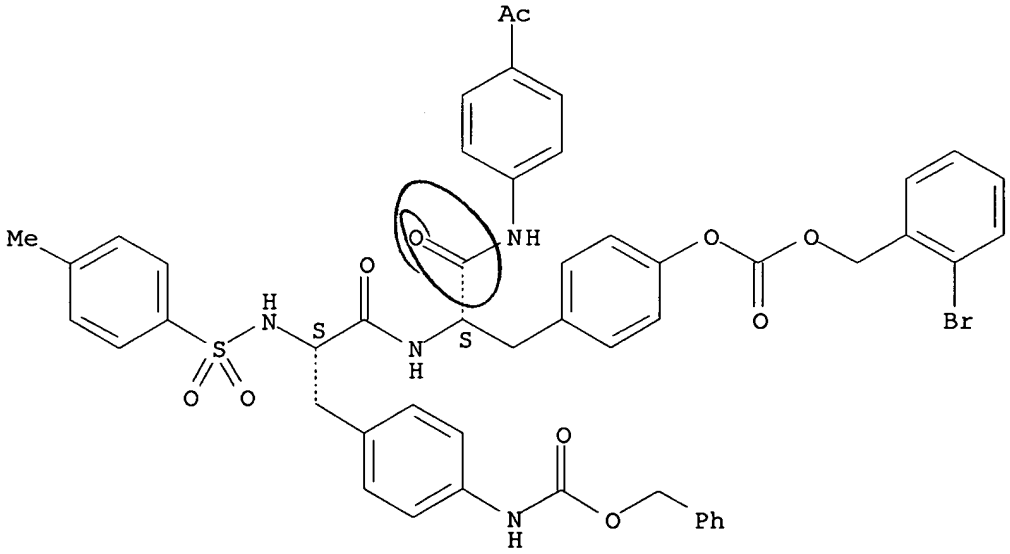
RN 152438-51-2 CAPLUS
CN L-Tyrosinamide, N2-[(4-methylphenyl)sulfonyl]-N6-[(phenylmethoxy)carbonyl]-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



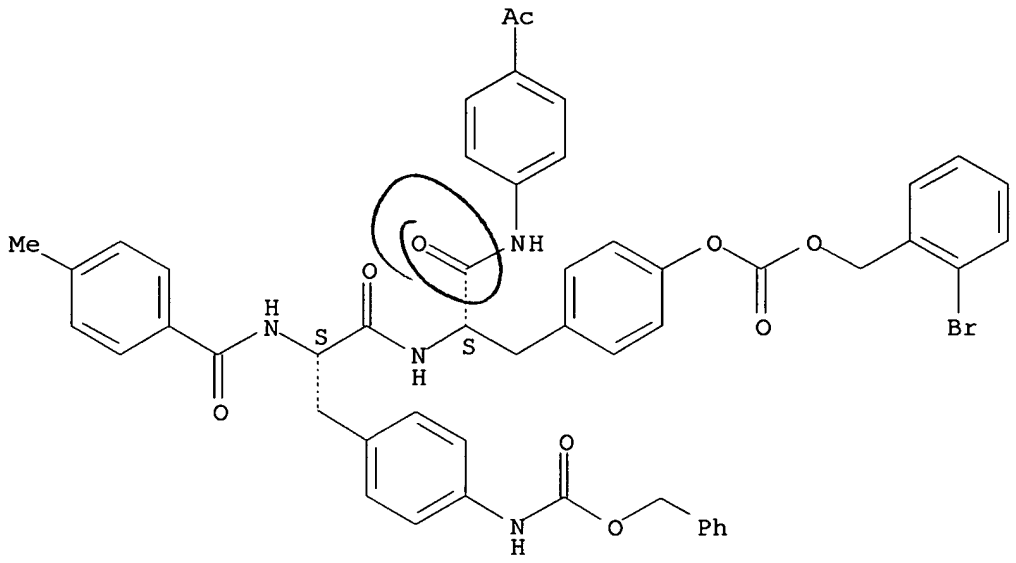
RN 152438-54-5 CAPLUS
CN L-Tyrosinamide, N-[(4-methylphenyl)sulfonyl]-4-[[(phenylmethoxy)carbonyl]amino]-L-phenylalanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

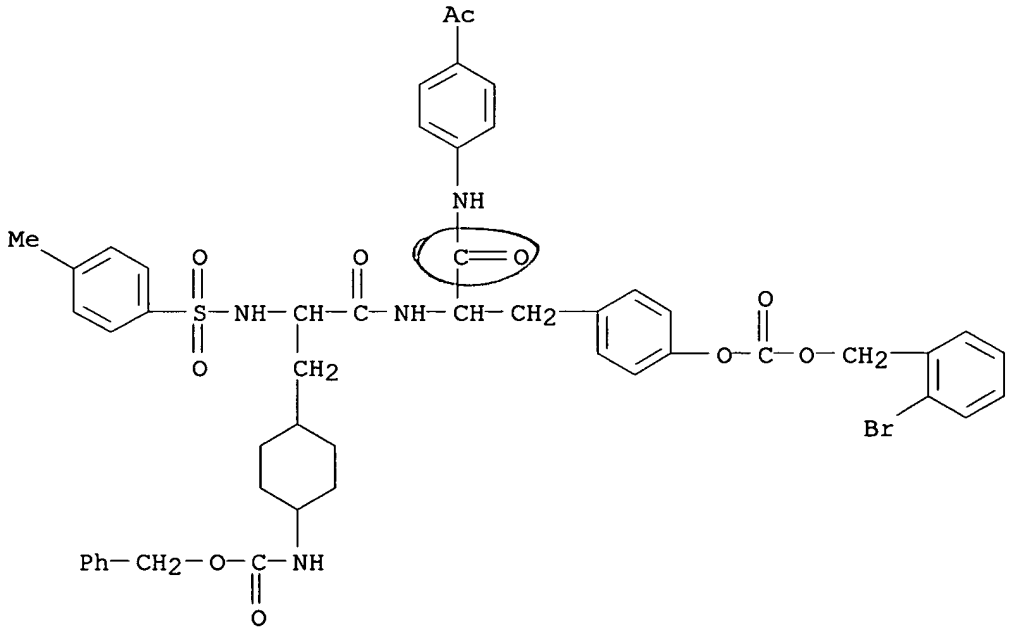


RN 152438-55-6 CAPLUS
CN L-Tyrosinamide, N-(4-methylbenzoyl)-4-[[(phenylmethoxy)carbonyl]amino]-L-phenylalanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

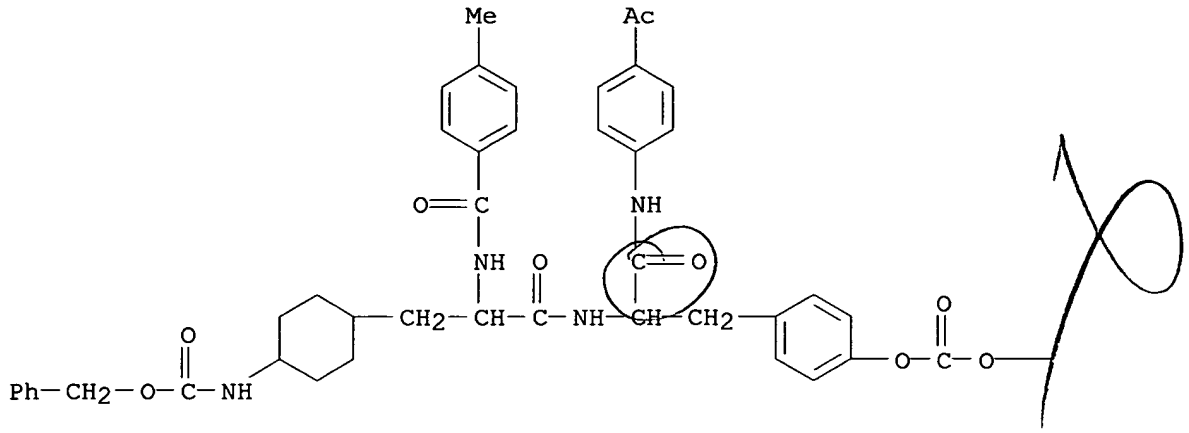


RN 152438-56-7 CAPLUS
CN L-Tyrosinamide, N-[(4-methylphenyl)sulfonyl]-3-[4-[[(phenylmethoxy)carbonyl]amino]cyclohexyl]-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), trans- (9CI) (CA INDEX NAME)

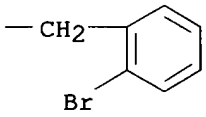


RN 152438-57-8 CAPLUS
CN L-Tyrosinamide, N-(4-methylbenzoyl)-3-[4-[[(phenylmethoxy)carbonyl]amino]cyclohexyl]-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), trans- (9CI) (CA INDEX NAME)

PAGE 1-A

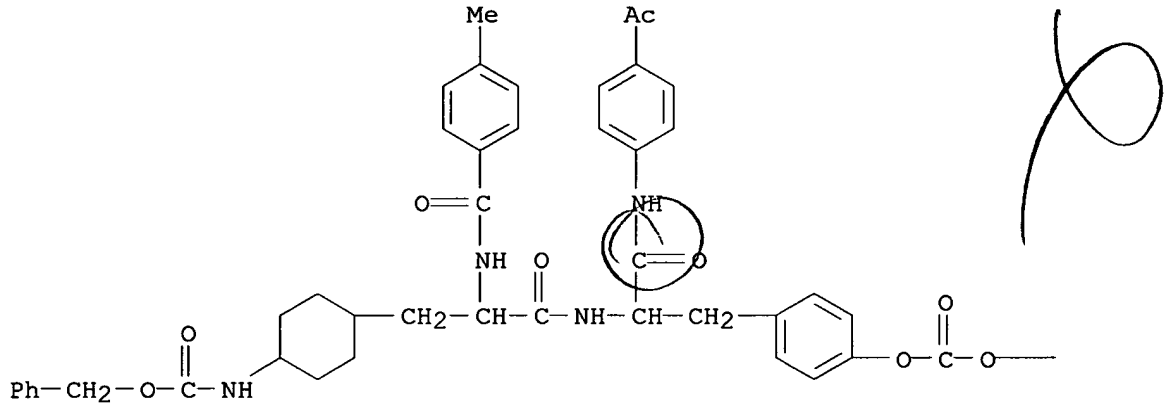


PAGE 1-B

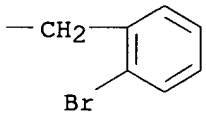


RN 152519-60-3 CAPLUS
CN L-Tyrosinamide, N-(4-methylbenzoyl)-3-[4-[[(phenylmethoxy)carbonyl]amino]cyclohexyl]-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), cis- (9CI) (CA INDEX NAME)

PAGE 1-A

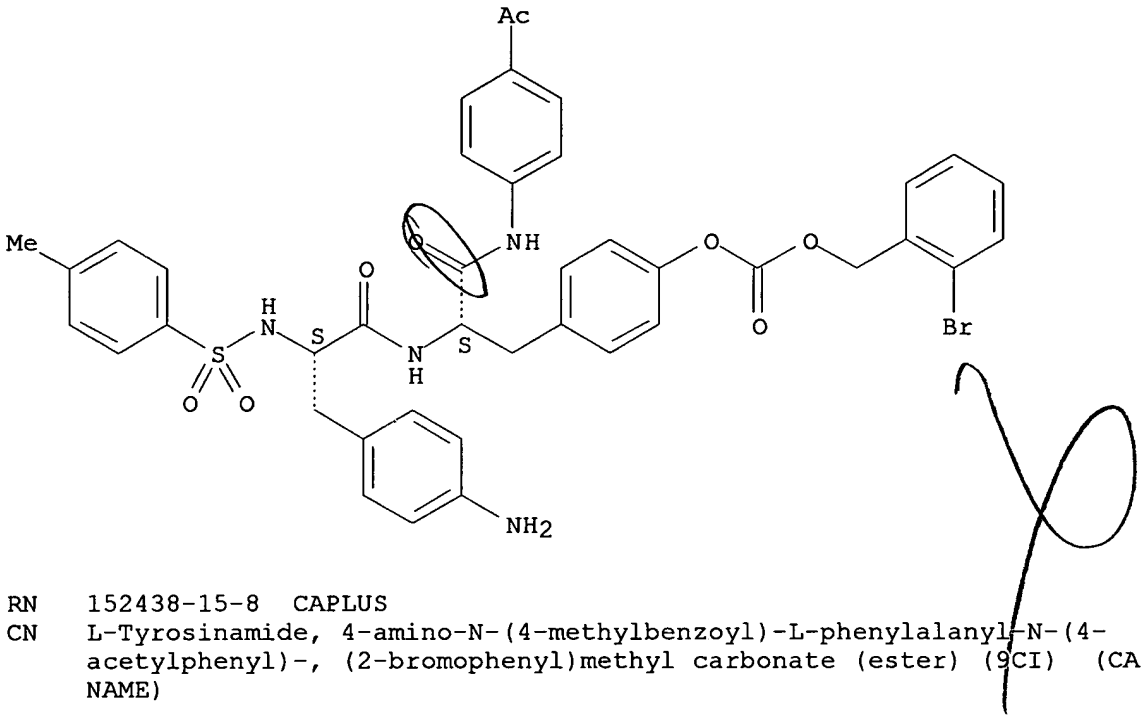


PAGE 1-B



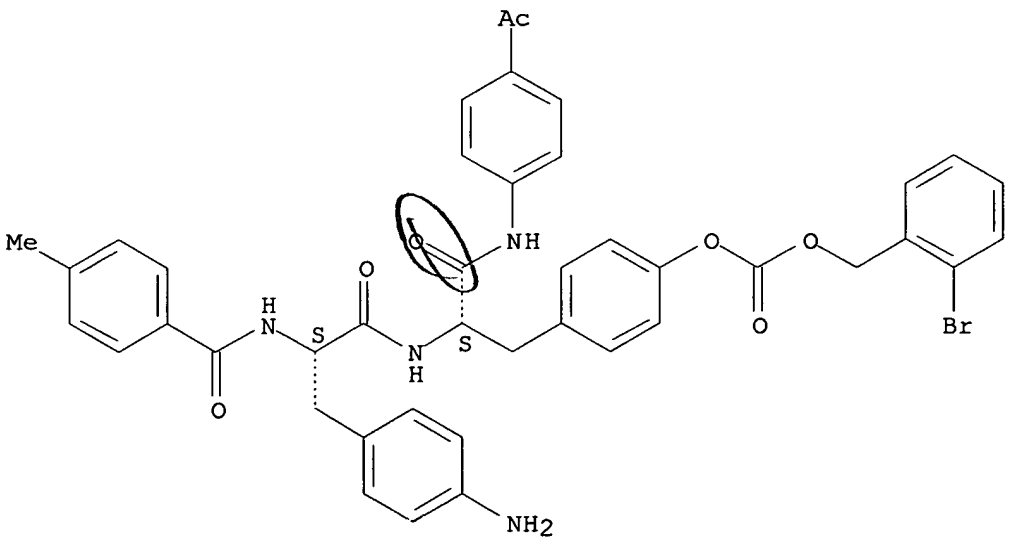
IT **152438-14-7P 152438-15-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and plasma kallikrein and plasmin inhibitory activities of)
RN 152438-14-7 CAPLUS
CN L-Tyrosinamide, 4-amino-N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



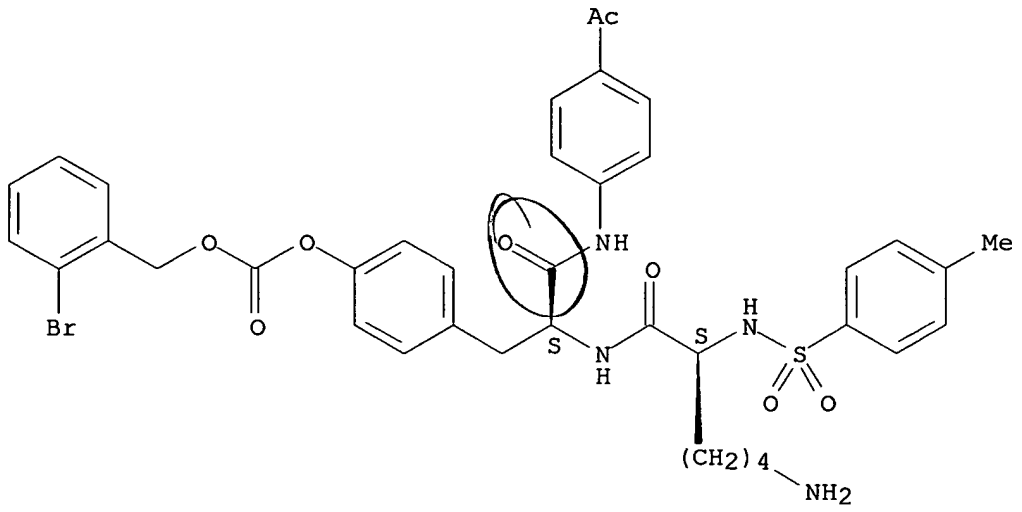
RN 152438-15-8 CAPLUS
CN L-Tyrosinamide, 4-amino-N-(4-methylbenzoyl)-L-phenylalanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



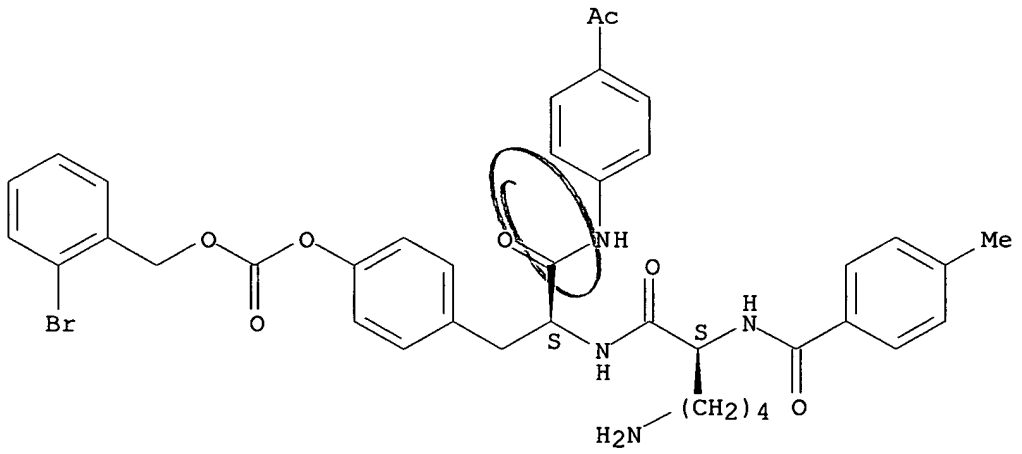
IT **152438-09-0P 152438-10-3P 152438-16-9P 152438-17-0P 152519-56-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and plasma kallikrein, plasmin, urokinase, and thrombin inhibitory activities of)
RN 152438-09-0 CAPLUS
CN L-Tyrosinamide, N2-[(4-methylphenyl)sulfonyl]-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

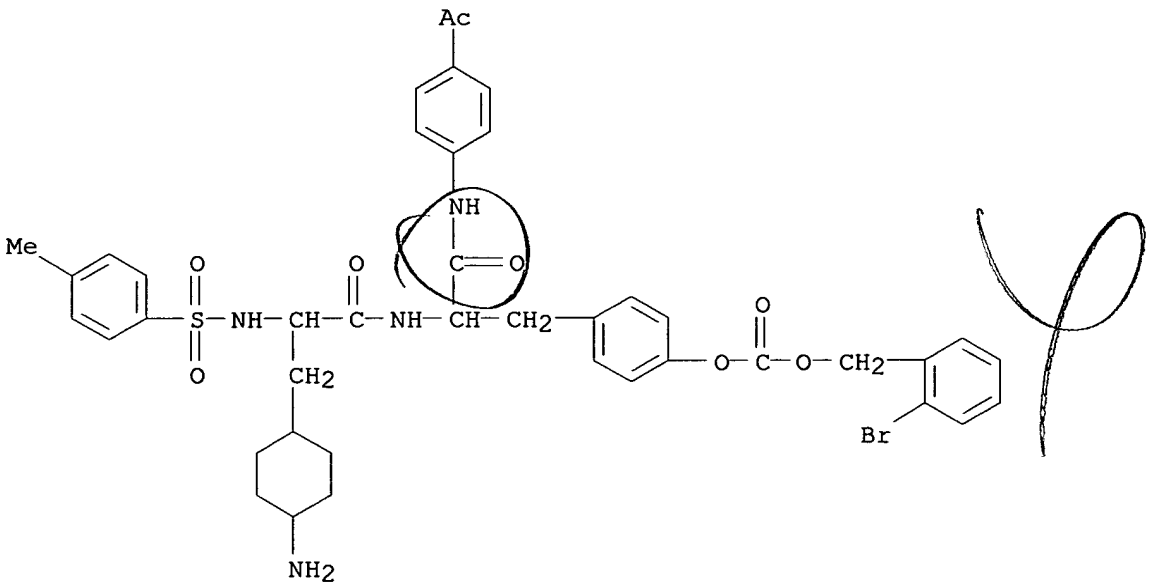


RN 152438-10-3 CAPLUS
CN L-Tyrosinamide, N2-(4-methylbenzoyl)-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

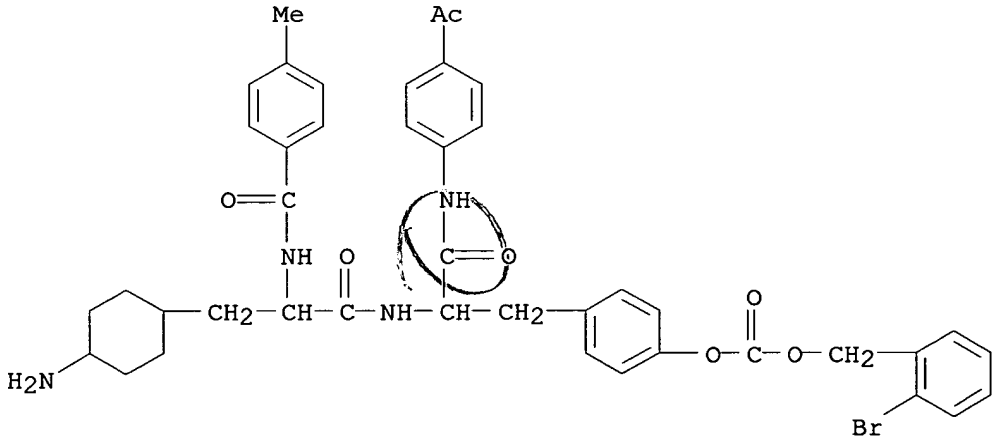
Absolute stereochemistry.



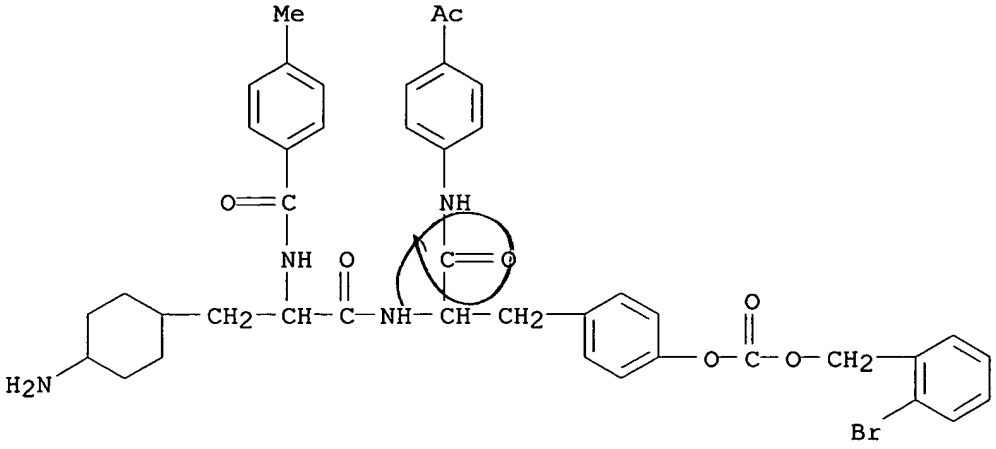
RN 152438-16-9 CAPLUS
CN L-Tyrosinamide, 3-(4-aminocyclohexyl)-N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), trans- (9CI) (CA INDEX NAME)



RN 152438-17-0 CAPLUS
CN L-Tyrosinamide, 3-(4-aminocyclohexyl)-N-(4-methylbenzoyl)-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), trans- (9CI) (CA INDEX NAME)

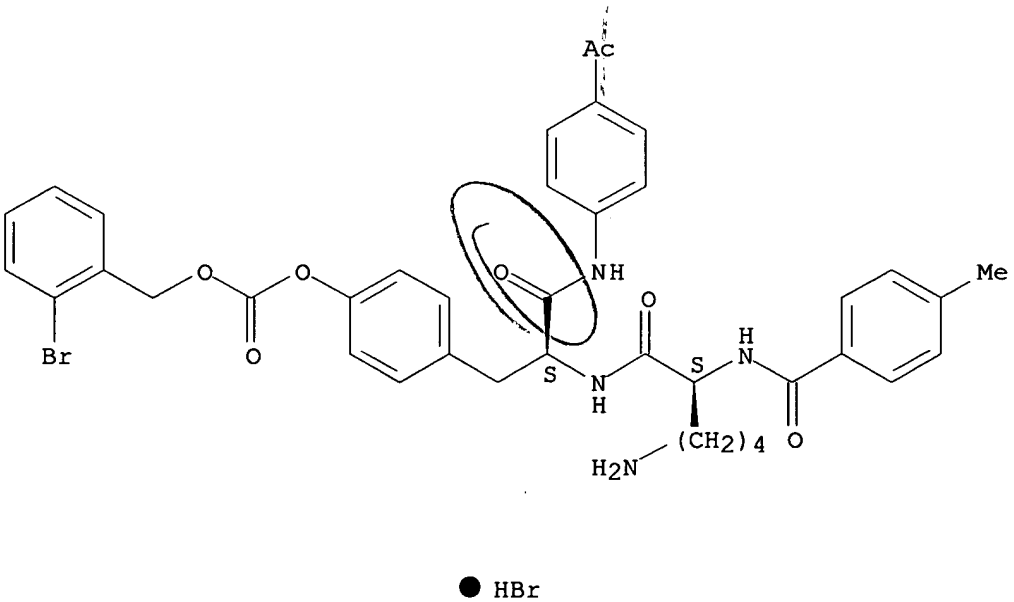


RN 152519-56-7 CAPLUS
CN L-Tyrosinamide, 3-(4-aminocyclohexyl)-N-(4-methylbenzoyl)-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), cis- (9CI) (CA INDEX NAME)



IT **120648-17-1P 120648-24-0P 152438-28-3P**
152438-29-4P 152520-66-6P 152520-67-7P
152610-68-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 120648-17-1 CAPLUS
CN L-Tyrosinamide, N2-(4-methylbenzoyl)-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

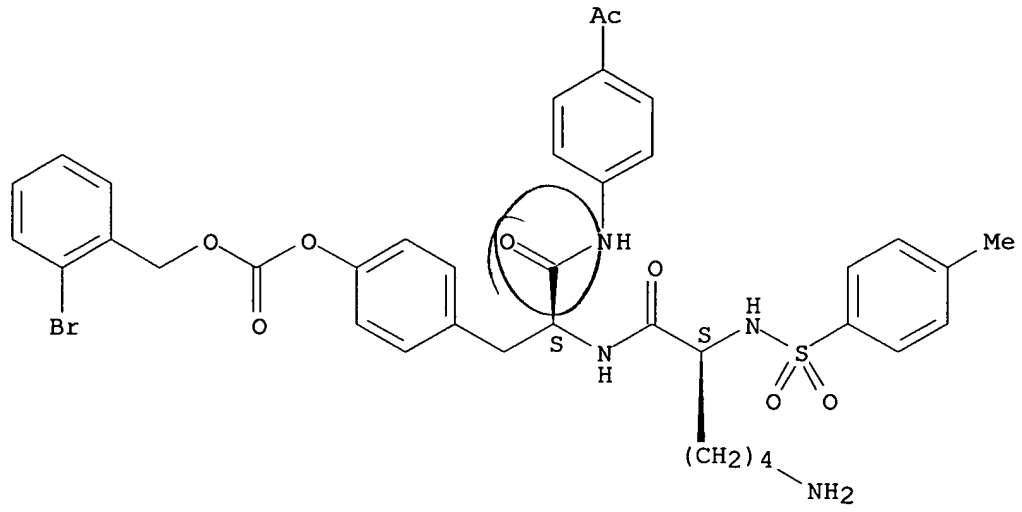


● HBr

RN 120648-24-0 CAPLUS
CN L-Tyrosinamide, N2-[(4-methylphenyl)sulfonyl]-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



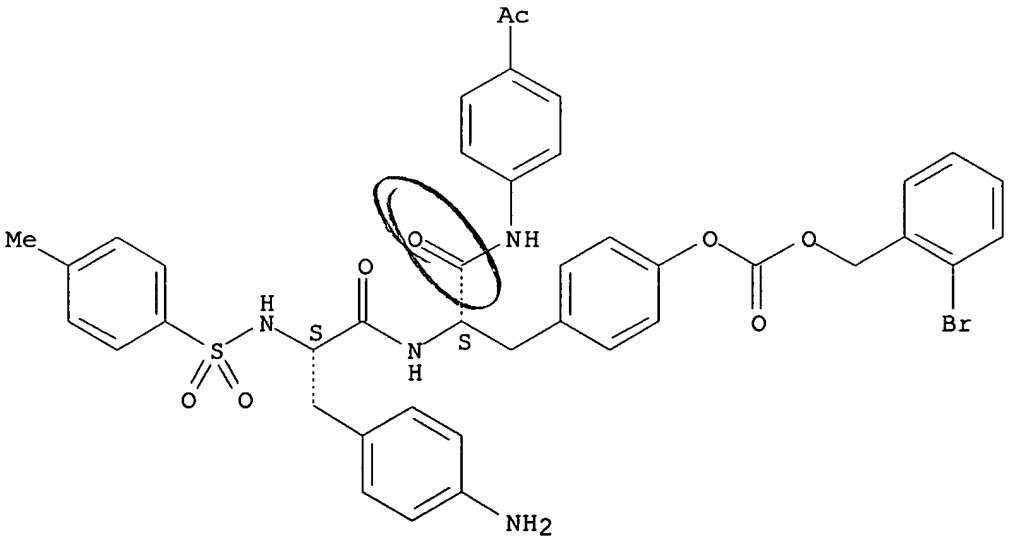
PAGE 2-A

● HBr

RN 152438-28-3 CAPLUS
CN L-Tyrosinamide, 4-amino-N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



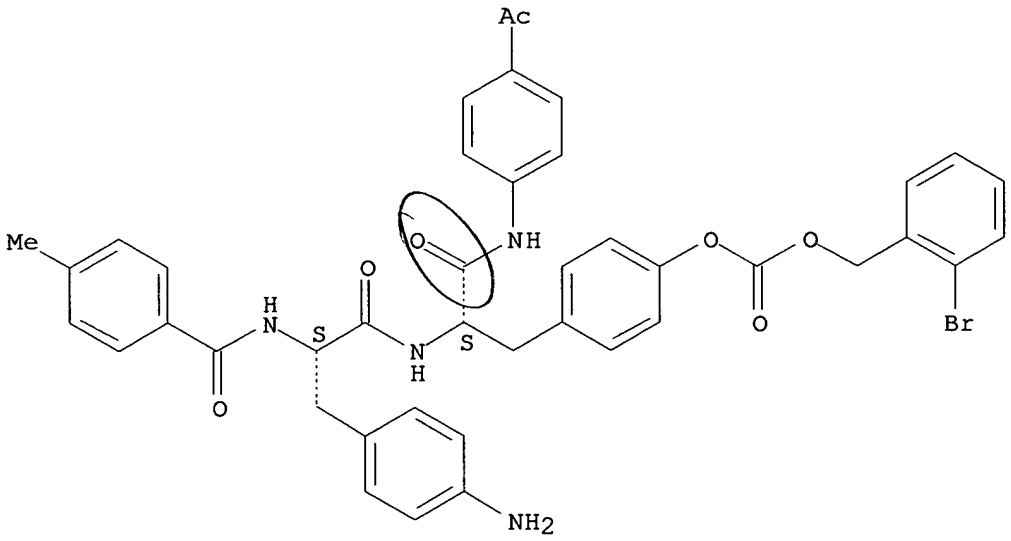
PAGE 2-A

● HBr

RN 152438-29-4 CAPLUS
CN L-Tyrosinamide, 4-amino-N-(4-methylbenzoyl)-L-phenylalanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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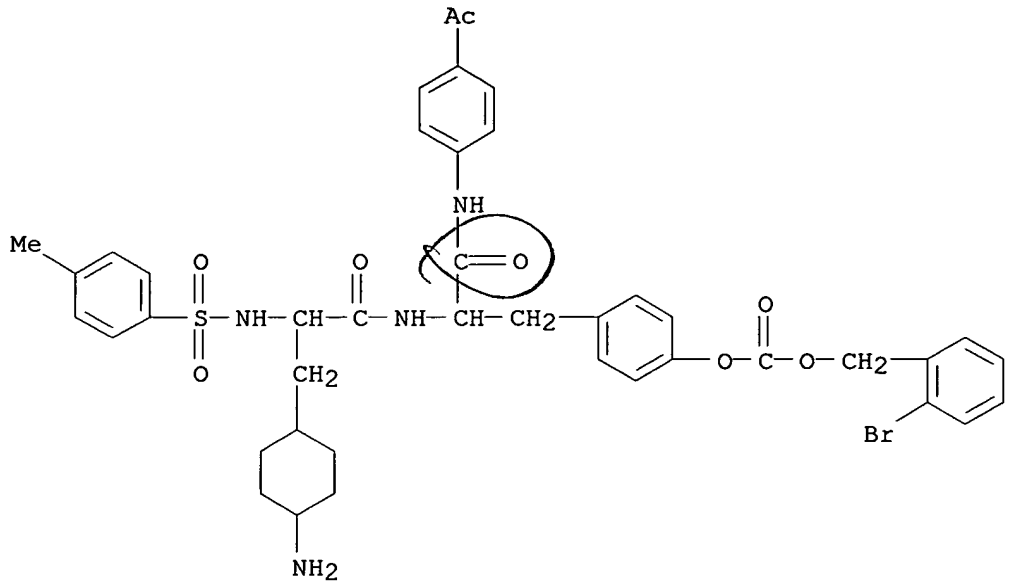
● HBr

RN 152520-66-6 CAPLUS
CN L-Tyrosinamide, 3-(4-aminocyclohexyl)-N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide, trans- (9CI) (CA INDEX NAME)

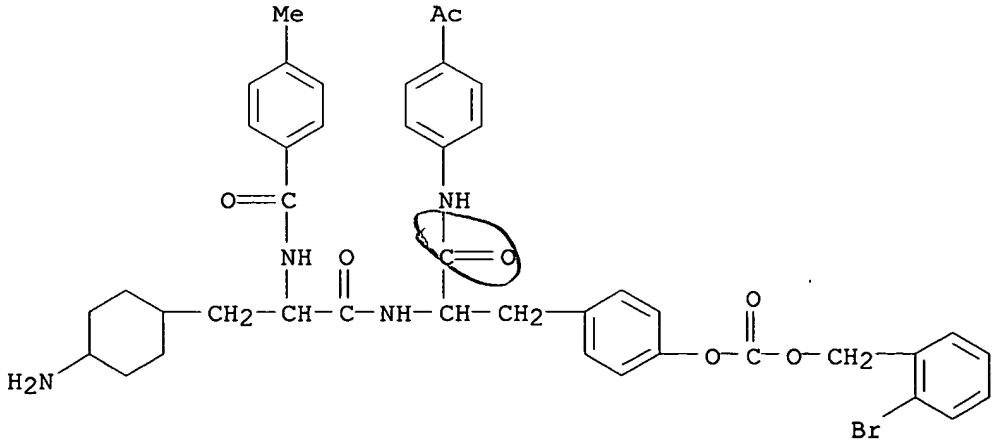
PAGE 1-A



PAGE 2-A

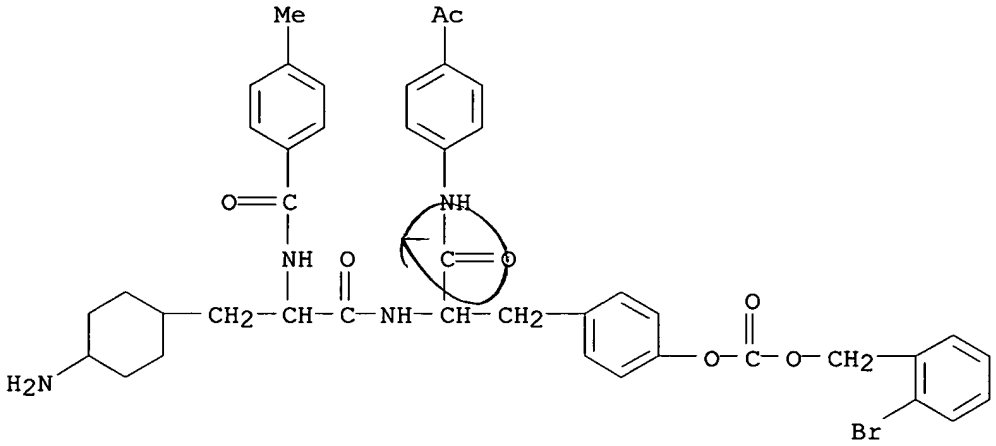
● HBr

RN 152520-67-7 CAPLUS
CN L-Tyrosinamide, 3-(4-aminocyclohexyl)-N-(4-methylbenzoyl)-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide, trans- (9CI) (CA INDEX NAME)



● HBr

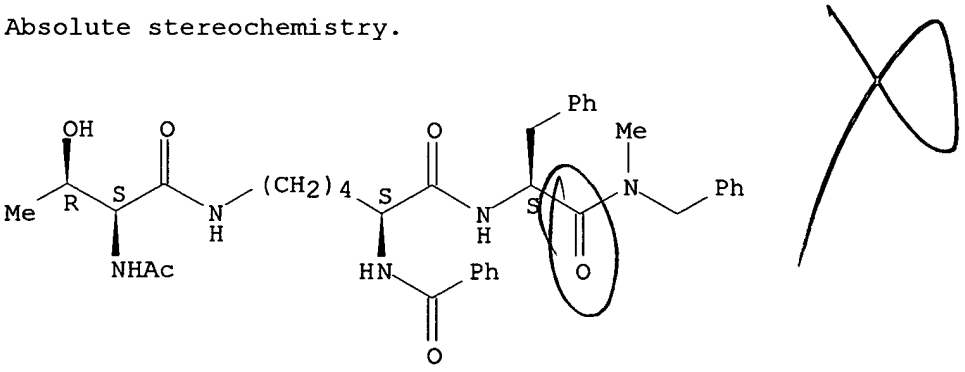
RN 152610-68-9 CAPLUS
CN L-Tyrosinamide, 3-(4-aminocyclohexyl)-N-(4-methylbenzoyl)-L-alanyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)



● HBr

L27 ANSWER 39 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1993:560780 CAPLUS
DN 119:160780
TI Studies on neurokinin antagonists. 3. Design and structure-activity relationships of new branched tripeptides N.alpha.-(substituted L-aspartyl, L-ornithyl, or L-lysyl)-N-methyl-N-(phenylmethyl)-L-phenylalaninamides as substance P antagonists
AU Hagiwara, Daijiro; Miyake, Hiroshi; Murano, Kenji; Morimoto, Hiroshi; Murai, Masako; Fujii, Takashi; Nakanishi, Isao; Matsuo, Masaaki
CS New Drug Res. Lab., Fujisawa Pharm. Co., Ltd., Osaka, 532, Japan
SO Journal of Medicinal Chemistry (1993), 36(16), 2266-78
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB As an extension of the study on discovering novel substance P (SP) antagonists, new branched tripeptides I (Bzl = benzyl), II, III (n = 3, 4) and IV (n = 3, 4) were designed by reconstructing the structure of the previously reported tripeptide SP antagonist Ac-Thr-D-Trp(CHO)-Phe-NMeBzl (V) (FR113680). The strategy for this design was based on the postulate that the dipeptide half D-Trp(CHO)-Phe-NMeBzl in V is essential for receptor recognition. Mol. modeling studies implied that these newly designed tripeptides could mimic the spatial orientations of the essential dipeptide structure. As expected, all of these compds. potently inhibited 3H-SP (1 nM) binding to guinea pig lung membranes in the 10-8 M range. The 1H-indol-3-ylcarbonyl derivs.were slightly more potent than the corresponding 1H-indol-2-ylcarbonyl derivs., as predicted by the mol. modeling studies. The structure-activity relationships studies on the selected 1H-indol-3-ylcarbonyl derivs. indicated that the threonine moiety at the side chain can be modified into a variety of structures without any significant loss of the activity. Furthermore, in the L-lysine series, even dipeptide compds. having nothing or a simple acyl group at the .epsilon.-amino group exhibited potent activity. These dipeptides belong to a new structural class of SP antagonist.
IT **150113-35-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 150113-35-2 CAPLUS
CN L-Phenylalaninamide, N6-(N-acetyl-L-threonyl)-N2-benzoyl-L-lysyl-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

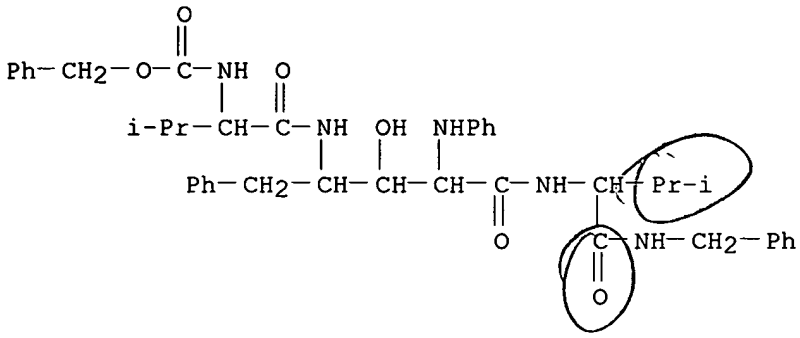
Absolute stereochemistry.



L27 ANSWER 40 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1993:473121 CAPLUS
DN 119:73121
TI 4-amino-3-hydroxycarboxylic acid derivatives
IN Billich, Andreas; Charpiot, Brigitte; Lehr, Philip; Scholz, Dieter
PA Sandoz Ltd., Switz.; Sandoz-Patent-G.m.b.H.
SO PCT Int. Appl., 49 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

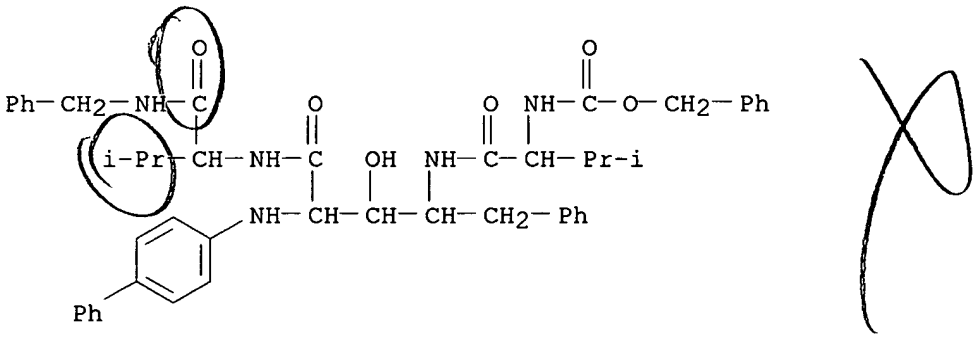
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9301166	A1	19930121	WO 1992-EP1471	19920630
	W: AU, CA, CS, FI, HU, JP, KR, NO, PL, RO, RU, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
	CA 2109326	AA	19930103	CA 1992-2109326	19920630
	AU 9221944	A1	19930211	AU 1992-21944	19920630
	EP 594656	A1	19940504	EP 1992-913821	19920630
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 07501786	T2	19950223	JP 1992-501937	19920630
	ZA 9204932	A	19940103	ZA 1992-4932	19920702
	CN 1088912	A	19940706	CN 1993-100562	19930101
PRAI	GB 1991-14261		19910702		
	GB 1991-23721		19911107		
	GB 1992-3884		19920224		
	WO 1992-EP1471		19920630		

OS MARPAT 119:73121
AB Title compds. I [A and B = bond or (un)substituted amino acid residue; R1 = H, amino protecting group, R6Y (R6 = H, alkyl, alkenyl, alkynyl, aryl, aralkyl, heteroaryl, etc.; Y = CO, NHCO,NHCS, SO2, OCO, OCS); R2 = amino acid side chain, alkyl, aralkyl, trimethylsilylmethyl, 2-thienylmethyl, etc.; R3 = alkyl, alkenyl, alkynyl, cycloalkyl, aryl, etc.; R4 = OR7 or NHR7 where R7 has the meaning indicated for R6; X = S or NR5 (R5 = H, Me, HCO, Ac) were prepd. antiviral agents, particularly HIV-1 proteinase inhibitors. Thus, Z-L-Val-OC6H4NO2-p (Z = PhCH2O2C) was coupled with L-phenylalaninol (Phe-ol) in the presence of Et3N in DMF to give Z-L-Val-L-Phe-ol, which underwent the Swern oxidn. with oxalyl chloride and DMSO to give the aldehyde, which underwent the Wittig reaction with Ph3P:CHCO2Et in toluene to give alkene II, which underwent epoxidn. with m-chloroperbenzoic acid in CH2Cl2 to give epoxide III. The epoxide of III was cleaved by PhCH2NH2 to give title compd. IV. I were measured for their ability to inhibit HIV proteinase and to inhibit the cellular HIV-induced cytopathic effect.
IT **148741-95-1P 148742-38-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as HIV proteinase inhibitor)
RN 148741-95-1 CAPLUS
CN Pentonamide, 2,4,5-trideoxy-4-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-N-[2-methyl-1-[[(phenylmethyl)amino]carbonyl]propyl]-5-phenyl-2-(phenylamino)-, [1(S),4(S)]- (9CI) (CA INDEX NAME)



RN 148742-38-5 CAPLUS

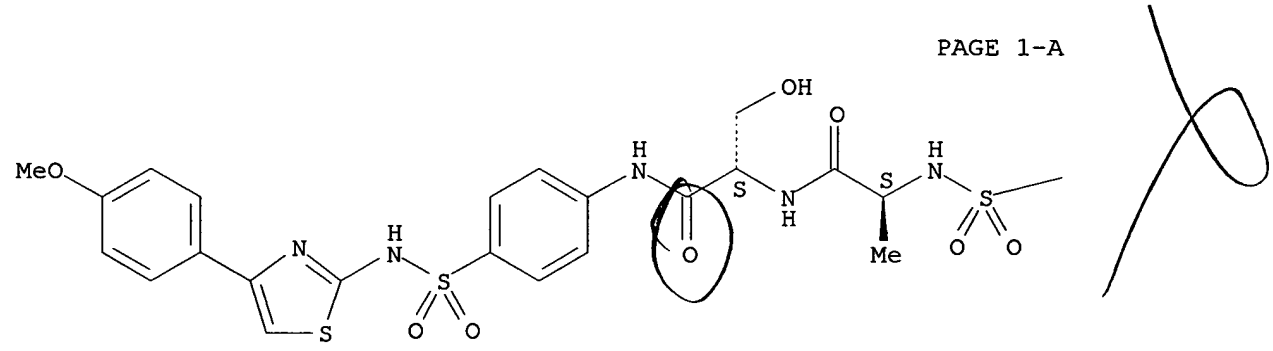
CN Pentonamide, 2-([1,1'-biphenyl]-4-ylamino)-2,4,5-trideoxy-4-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-N-[2-methyl-1-[[(phenylmethyl)amino]carbonyl]propyl]-5-phenyl-, [1(S),4(S)]- (9CI) (CA INDEX NAME)



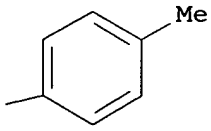
L27 ANSWER 41 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1993:428571 CAPLUS
DN 119:28571
TI Sulfanilamidothiazole-amino acid derivatives
AU Gommaa, A. M.
CS Fac. Sci., Al-Azhar Univ., Nasr, Egypt
SO Al-Azhar Bulletin of Science (1991), 2(1), 35-41
CODEN: ABSCE7; ISSN: 1110-2535
DT Journal
LA English
AB Title compds. I (R = tosyl, phthalyl; X = Gly, Ala, Ser, Val, Leu, Phe) were prepd. by std. coupling of the amino acid derivs. with 2-sulfanilamido-4-(4-methoxyphenyl)thiazole in the presence of DCC. Hydrazinolysis of the phthalyl derivs. gave the corresponding free amino derivs. I (R = H), which underwent further peptide coupling to give dipeptides I (R = N-tosylalanine N-phthalylserine). Some of the prepd. compds. I were active bactericides and fungicides.
IT **146038-16-6P 146038-17-7P 146038-18-8P 146038-19-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and bactericidal and fungicidal activity of)
RN 146038-16-6 CAPLUS
CN L-Serinamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



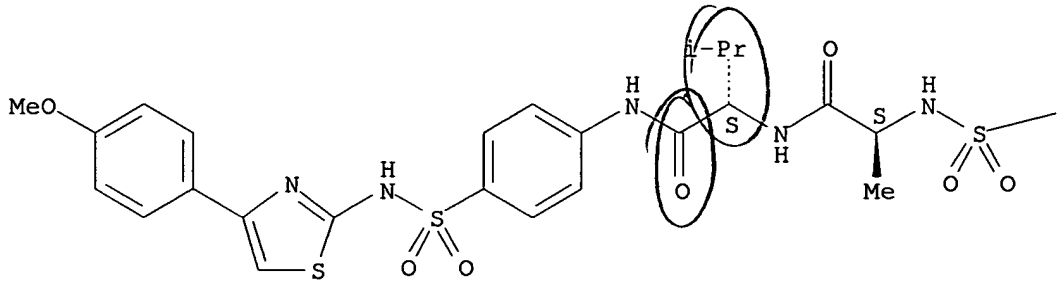
PAGE 1-B



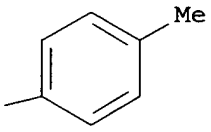
RN 146038-17-7 CAPLUS
CN L-Valinamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



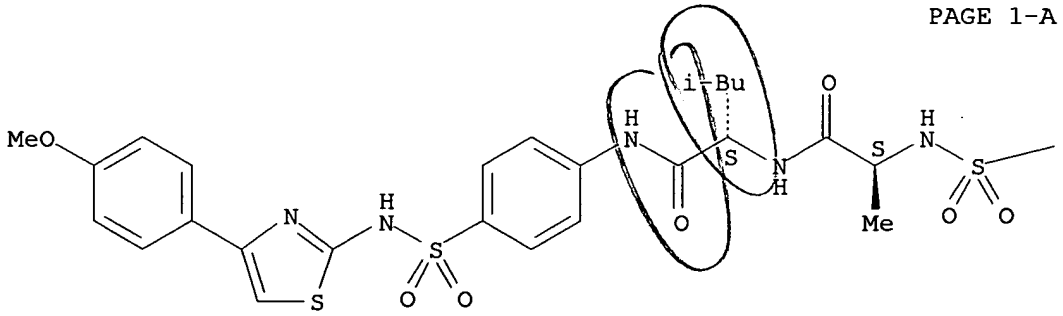
PAGE 1-B



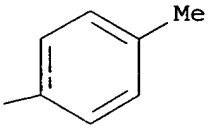
RN 146038-18-8 CAPLUS
CN L-Leucinamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



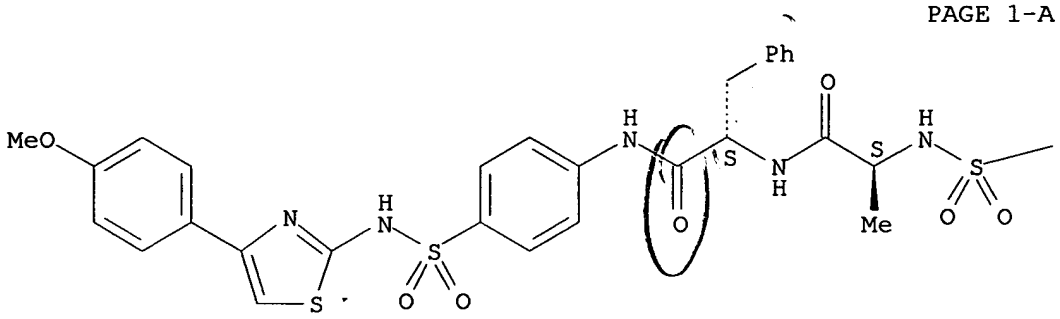
PAGE 1-B



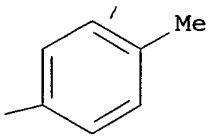
RN 146038-19-9 CAPLUS
CN L-Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



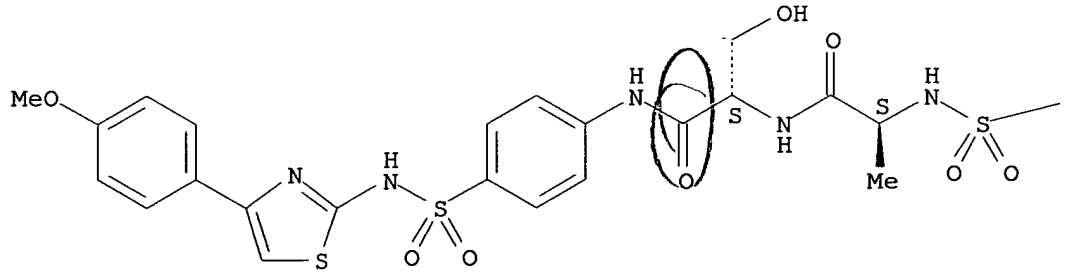
PAGE 1-B



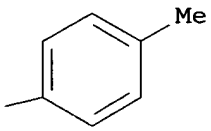
L27 ANSWER 42 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1993:125015 CAPLUS
DN 118:125015
TI Synthesis of some biologically active substituted thiazole derivatives
AU Gommaa, A. M.
CS Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SO Izvestiya po Khimiya (1991), 24(3), 448-52
CODEN: IZKHDX; ISSN: 0324-0401
DT Journal
LA English
AB Condensation of 2-sulfanilamido-4-(p-methoxyphenyl)thiazole (I; R = H) with N-tosyl or N-phthaloyl amino acids gave the corresponding I (R = N-protected amino acid residue). Hydrazinolysis of I (R = N-phthaloyl amino acid residue) gave the unprotected amino acid derivs. I (R = H-Gly, H-Ala, H-Ser, H-Val, H-Leu, H-Phe) (II). Coupling of II with N-tosyl and N-phthaloyl amino acids with DCC gave dipeptide derivs. Some of the prepd. compds. were active bactericides and fungicides.
IT **146038-16-6P 146038-17-7P 146038-18-8P**
146038-19-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and bactericidal and fungicidal activity of)
RN 146038-16-6 CAPLUS
CN L-Serinamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



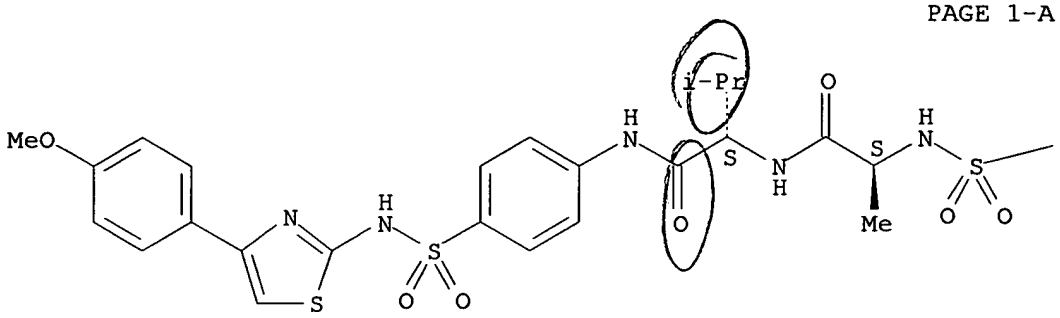
PAGE 1-B



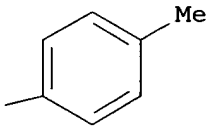
RN 146038-17-7 CAPLUS
CN L-Valinamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



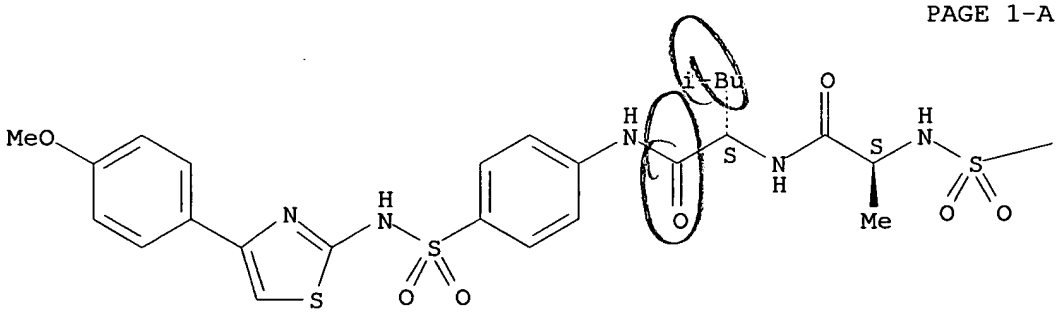
PAGE 1-B



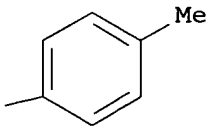
RN 146038-18-8 CAPLUS
CN L-Leucinamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



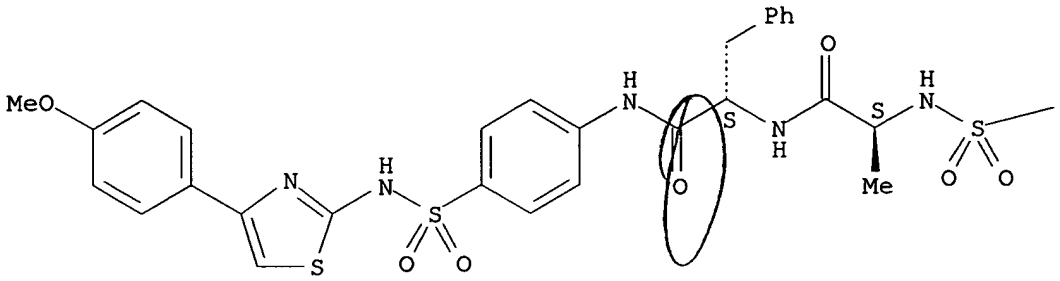
PAGE 1-B



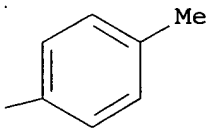
RN 146038-19-9 CAPLUS
CN L-Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]-L-alanyl-N-[4-[[[4-(4-methoxyphenyl)-2-thiazolyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

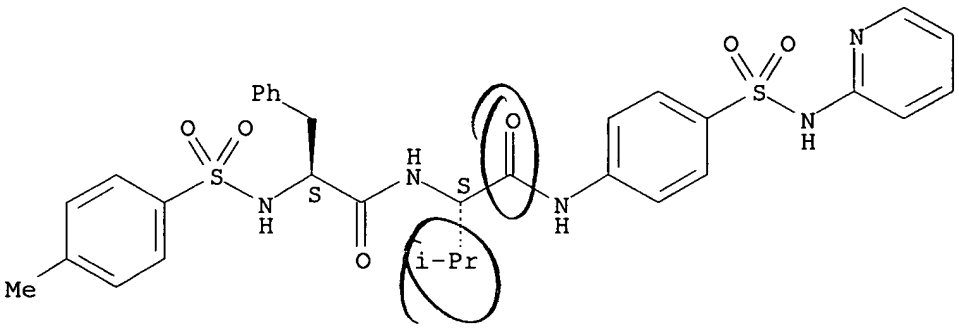


PAGE 1-B



L27 ANSWER 43 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1993:81392 CAPLUS
DN 118:81392
TI Synthesis of some sulfapyridine- and 2-(pyridylsulfamoyl)cinnamoyl-amino acid derivatives
AU Badie, M. F.; Ibrahim, T. M.; Shedid, S. A.; El-Naggar, A. M.
CS Fac. Sci., Al-Azhar Univ., Nasr, Egypt
SO Proceedings of the Indian National Science Academy, Part A: Physical Sciences (1992), 58(3), 253-60
CODEN: PIPSBD; ISSN: 0370-0046
DT Journal
LA English
AB The title compds. I (R = N-phthalylamino acid, N-tosylamino acid, R1 = H, NO2) and II (R2 = amino acid Me ester, amino acid hydrazide) were prepd. by condensation of the corresponding amino acid deriv. with the appropriate sulfapyridine or (pyridylsulfamoyl)cinnamic acid. Bromination of II (R2 = amino acid Me ester) gave the corresponding dibromides. I were active against a no. of bacteria and fungi, while I (R = free amino acid) and II were inactive.
IT **145764-34-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 145764-34-7 CAPLUS
CN L-Valinamide, N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-[4-[(2-pyridinylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

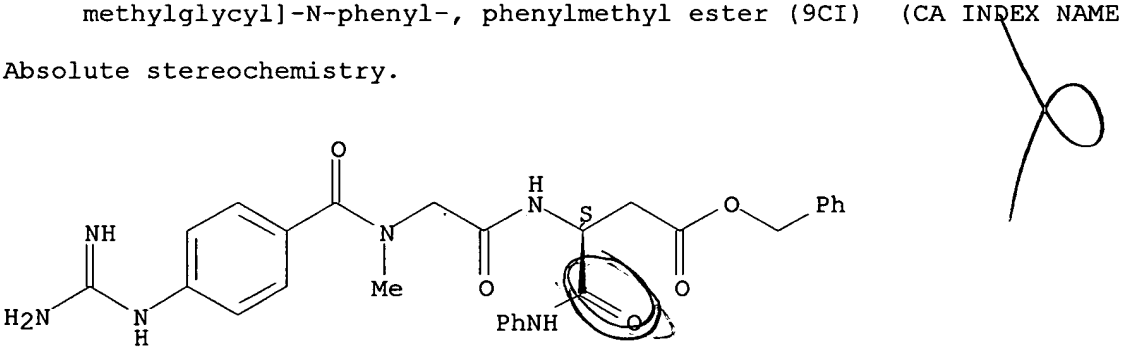


L27 ANSWER 44 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1993:7397 CAPLUS
DN 118:7397
TI Anti-aggregatory peptides containing an aromatic ester or amide
IN Ali, Fadia El Fehail; Bondinell, William Edward; Ku, Thomas Wen Fu; Samanen, James Martin
PA SmithKline Beckman Corp., USA
SO PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9213552	A1	19920820	WO 1992-US999	19920205
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE				
EP 570507	A1	19931124	EP 1992-906660	19920205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE				
JP 06505978	T2	19940707	JP 1992-506448	19920205
PRAI US 1991-650527		19910205		
WO 1992-US999		19920205		

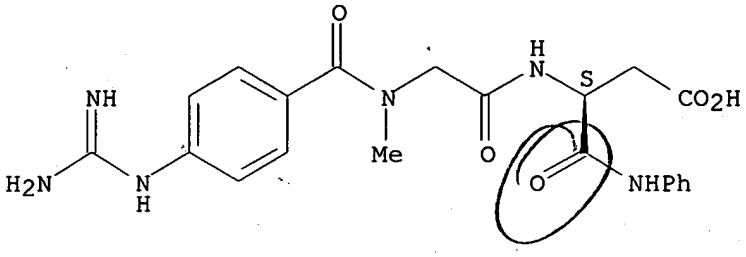
OS MARPAT 118:7397
AB The title compds. are prepd. for inhibiting platelet aggregation. E.g., I and II were prepd. by std. peptide synthesis and parenteral dosage unit compns. contg. I or II were prepd.
IT **144838-06-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrogenation of)
RN 144838-06-2 CAPLUS
CN L-.alpha.-Asparagine, N2-[N-[4-[(aminoiminomethyl)amino]benzoyl]-N-methylglycyl]-N-phenyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



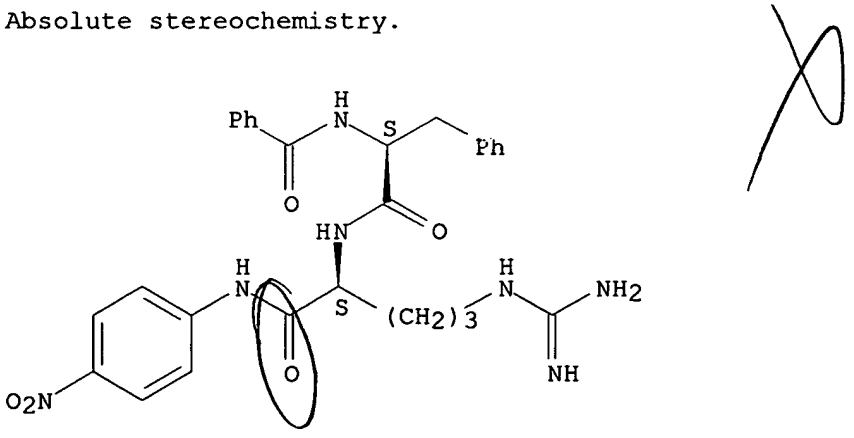
IT **144838-63-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as blood platelet aggregation inhibitor)
RN 144838-63-1 CAPLUS
CN L-.alpha.-Asparagine, N2-[N-[4-[(aminoiminomethyl)amino]benzoyl]-N-methylglycyl]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



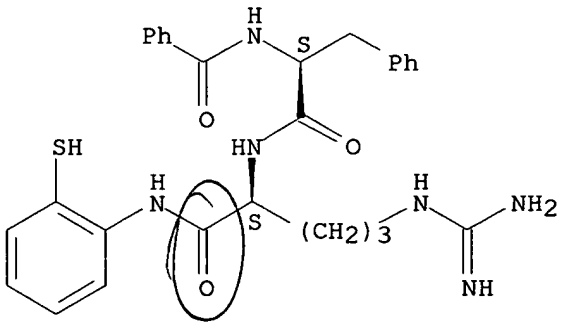
L27 ANSWER 45 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1990:547900 CAPLUS
DN 113:147900
TI Hydrolysis of synthetic peptides and natural substrates by plasma kallikrein and its light chain
AU Motta, Guacyara; Sampaio, Misako U.; Sampaio, Claudio A. M.
CS Dep. Bioquim., Esc. Paulista Med., Sao Paulo, 04034, Brazil
SO Advances in Experimental Medicine and Biology (1989), 247B(Kinins 5, Pt. B), 239-42
CODEN: AEMBAP; ISSN: 0065-2598
DT Journal
LA English
AB The enzymic properties of human blood plasma .alpha.- and .beta.-kallikreins and the light chain were compared. The activity of all forms of kallikrein was measured with tosylarginine Me ester (TAME), after active site titrn., and the esterolytic activity was found to be higher for the light chain when compared to both .alpha.-kallikrein and .beta.-kallikrein, being, resp., 275, 72, and 101 .mu.mols TAME hydrolyzed/min/mg enzyme. With dipeptides, an increased efficiency as measured by the kcat/Km ratio was due chiefly to a higher catalytic activity; with tripeptides there was also an important contribution of Km that was lower for light chain when compared to the other 2 enzyme forms. One possible explanation for this difference would be an easier diffusion of the substrate, in the absence of the enzyme heavy chain. The assocn. of free heavy and light chains is not spontaneous since no changes in the kinetic parameters were detected when heavy chain was added to light chain solns. The heavy chain is fundamental for the assocn. of kallikrein to kininogen, and only 1 cleavage on the heavy chain impairs the efficiency of bradykinin release; furthermore, the heavy chain does not seem to be necessary for nonspecific cleavages of kininogen, as seen by SDS-PAGE but only for bradykinin generation. The kinin releasing activity was present mostly in .alpha.-kallikrein; .beta.-kallikrein activity toward high-mol.-wt. kininogen was 25% of that obsd. for .alpha.-kallikrein; light chain did not release bradykinin from kininogen, although all enzyme forms could cleave high-mol.-wt. kininogen, as seen by product anal. of these incubates performed by SDS-PAGE.
IT **103418-68-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with kallikrein multiple forms of human, kinetics of)
RN 103418-68-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



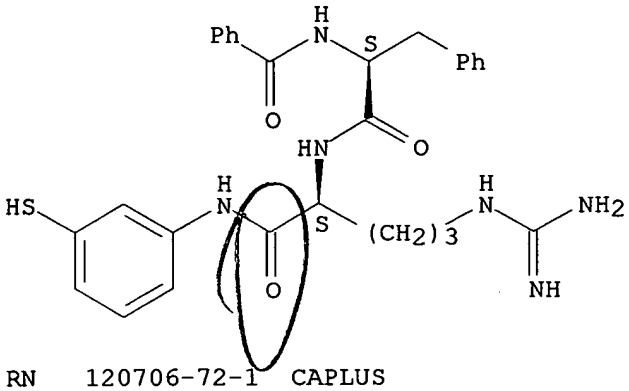
L27 ANSWER 46 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1990:473561 CAPLUS
DN 113:73561
TI Substrate specificity and inhibition of Pseudomonas aeruginosa alkaline protease
AU Morimoto, Takashi; Nishino, Norikazu; Fujimoto, Tsutomu; Yamamoto, Tetsuro
CS Dep. Appl. Chem., Kyushu Inst. Technol., Kitakyushu, 804, Japan
SO Peptide Chemistry (1990), Volume Date 1989, 27th, 387-90
CODEN: PECHDP; ISSN: 0388-3698
DT Journal
LA English
AB The alk. proteinase of P. aeruginosa was identified as a C-type metalloproteinase similar to the 56K proteinase of Serratia on the basis of specificity studies with fluorogenic peptide substrates and peptidylmercaptoanilide inhibitors kinetic parameters (Km, kcat, kcat/Km, and Ki values) are reported and structure-activity relations of the substrates and inhibitors are discussed.
IT **120706-69-6 120706-71-0 120706-72-1**
120706-73-2 120706-74-3 120706-75-4
120706-76-5 120706-77-6 120706-78-7
128533-12-0
RL: BIOL (Biological study)
(alk. proteinase of Pseudomonas aeruginosa inhibition by, kinetics of, structure in relation to)
RN 120706-69-6 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(2-mercaptophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



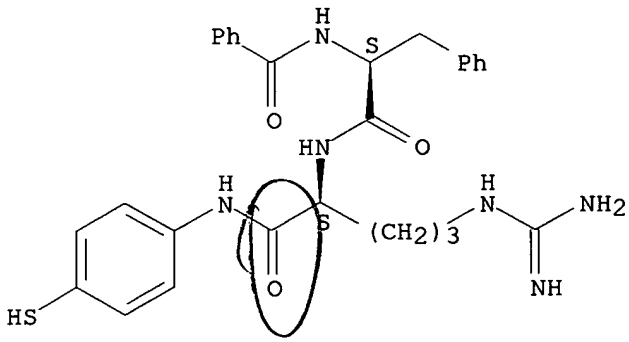
RN 120706-71-0 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(3-mercaptophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



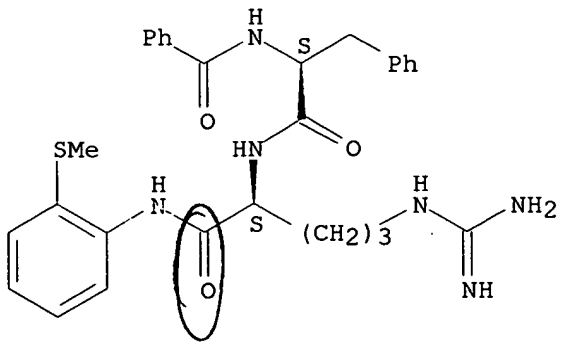
RN 120706-72-1 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-mercaptophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



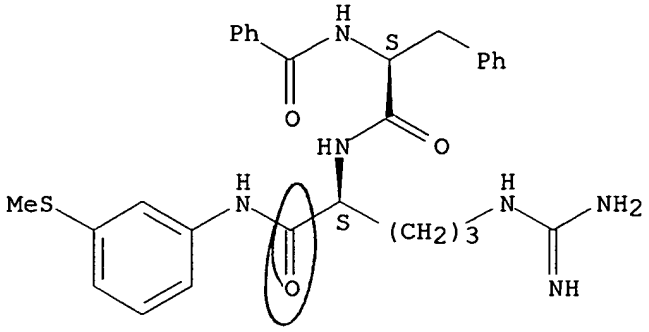
RN 120706-73-2 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[2-(methylthio)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



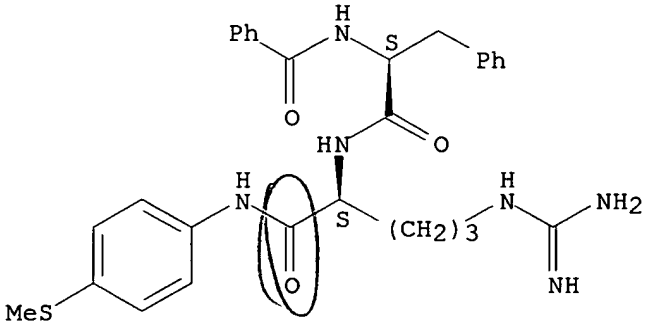
RN 120706-74-3 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[3-(methylthio)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



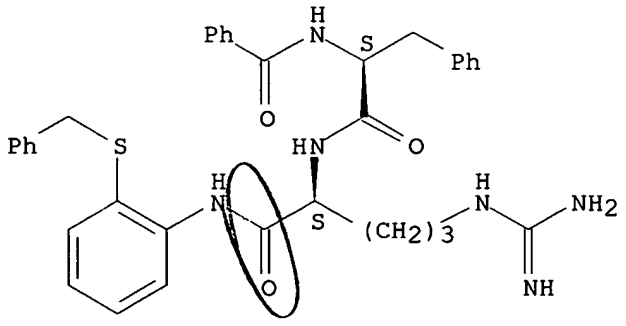
RN 120706-75-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



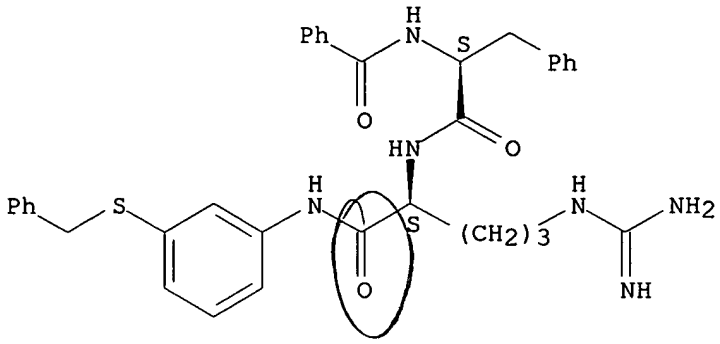
RN 120706-76-5 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[2-[(phenylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



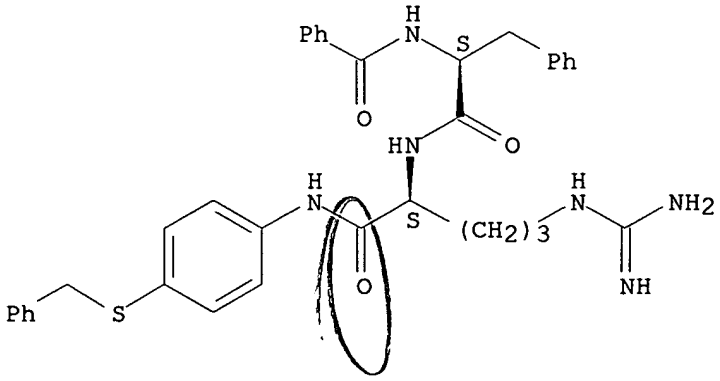
RN 120706-77-6 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[3-[(phenylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



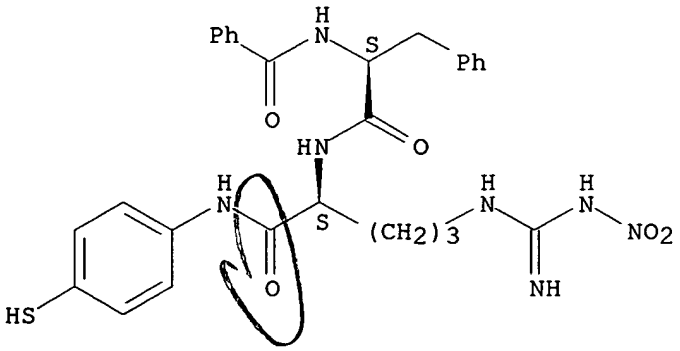
RN 120706-78-7 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[4-[(phenylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 128533-12-0 CAPLUS
CN L-Ornithinamide, N-benzoyl-L-phenylalanyl-N5-[imino(nitroamino)methyl]-N-(4-mercaptophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

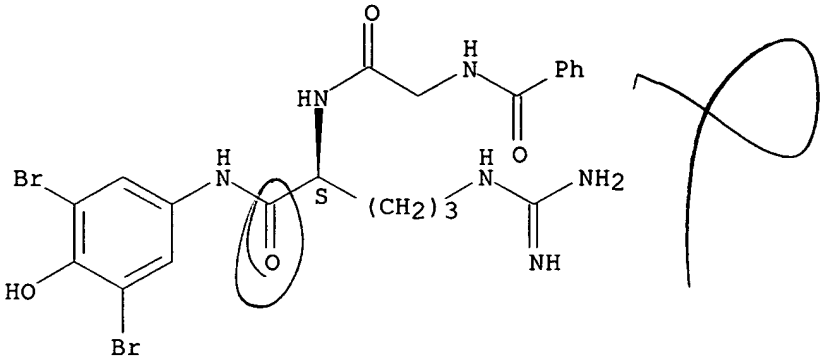


L27 ANSWER 47 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1990:154777 CAPLUS
DN 112:154777
TI Composition or kit containing peptide substrates for testing periodontal diseases by determining peptidase-like enzymic activity
IN Suido, Hirohisa; Miike, Akira; Hasegawa, Kenji; Kayahara, Norihiko; Eguchi, Toru; Tatano, Toshio; Nakashima, Koichi
PA Sunstar, Inc., Japan; Kyowa Medex Co., Ltd.
SO Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 325472	A2	19890726	EP 1989-300533	19890120
	EP 325472	A3	19900620		
	EP 325472	B1	19930428		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 02000499	A2	19900105	JP 1988-331988	19881228
	JP 06050995	B4	19940706		
	AT 88759	E	19930515	AT 1989-300533	19890120
	ES 2055029	T3	19940816	ES 1989-300533	19890120
	CA 1332347	A1	19941011	CA 1989-588832	19890120
	US 5223404	A	19930629	US 1991-639742	19910111
PRAI	JP 1988-10241		19880120		
	JP 1988-331988		19881228		
	US 1989-298965		19890119		
	EP 1989-300533		19890120		

OS MARPAT 112:154777
AB The title compn. or kit comprises (1) peptide derivs. X-T-Pro-Y and/or X-Z-Arg-Y (X = H, amino protecting group; Y is a residue of a compd. capable of increasing the oxidn. rate of a chromogen with an oxidase in the presence of O; T, Z = amino acid, peptide contg. 0-4 amino acids or their protected derivs.); (2) a chromogen; and (3) an oxidase. The enhancer residue Y may be an aniline deriv. Saliva samples from healthy subjects and patients with periodontitis and juvenile periodontitis were centrifuged and the supernatants were tested for hydrolytic activity using N-carbobenzoxy-glycyl-arginine-DIHA (DIHA = 3,5-diiodo-4-hydroxyanilinyl) and N-benzoyl-arginyl-glycyl-phenylalanyl-proline-DIHA, alone or in combination, as substrates, ascorbate oxidase, and I. The diseased group showed .gtorsim.1.5 times higher activity than the healthy group when both substrates were used. The values were 10 times higher than those of a conventional method.
IT **126152-05-4**
RL: ANST (Analytical study)
(as substrate, in peptidase assay for periodotal disease diagnosis)
RN 126152-05-4 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(3,5-dibromo-4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

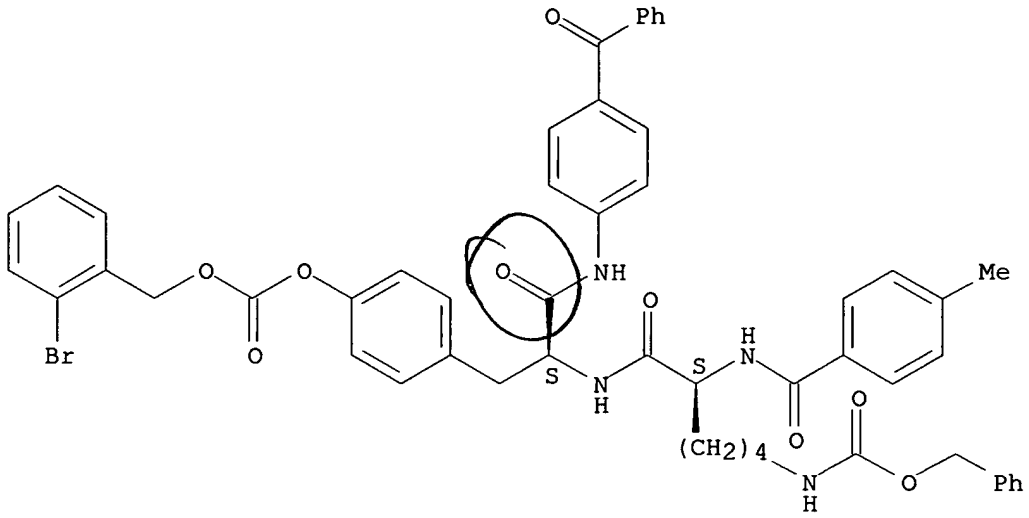


L27 ANSWER 48 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1989:232091 CAPLUS
DN 110:232091
TI Protease inhibitors containing phenylalanine derivatives
IN Akiyoshi, Okamoto; Okada, Yoshio; Okumiya, Akiko; Teno, Naoki; Wanaka, Keiko; Naito, Taketoshi
PA Showa Denko K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 63243095	A2	19881007	JP 1987-74459	19870330
PRAI JP 1987-74459		19870330		

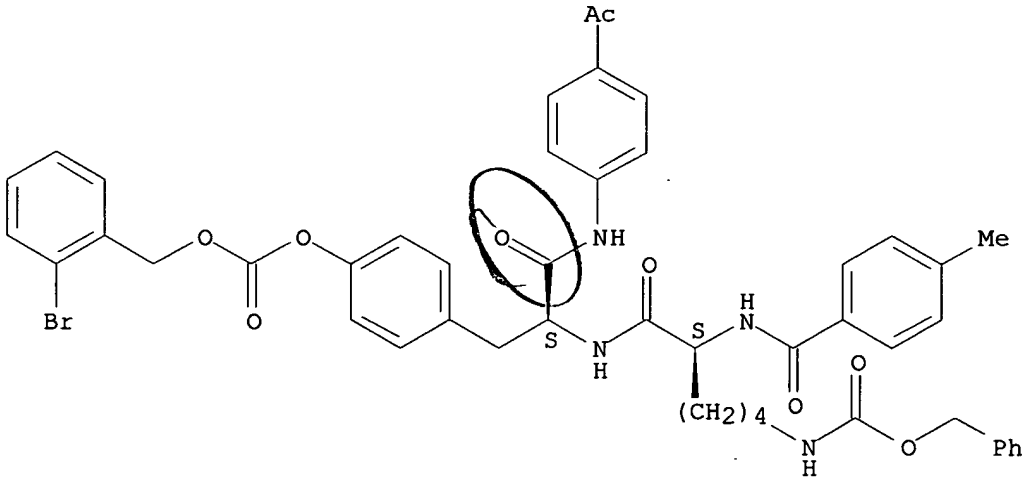
OS MARPAT 110:232091
AB Lysylphenylalanine derivs. [I; X = alkanoyl, (substituted) benzoyl, naphthoyl, fluorenylalkoxycarbonyl, (substituted) phenylsulfonyl, naphthysulfonyl; Y = alkyl, Ph; Z = (substituted) phenylalkoxycarbonyl; n = 0, 1] and their pharmaceutically acceptable salts are useful as protease inhibitors. L-Tyrosine was reacted with o-BrC6H4CH2O2CCl to give 4-(2-bromobenzyloxycarbonyloxy)-L-phenylalanine, which was N-protected with Me3CO2C and reacted with p-H2NC6H4COMe to give N-(tert-butoxycarbonyl)-4-(2-bromobenzyloxycarbonyloxy)-L-phenylalanine 4-acetylanilide. The hydrochloride salt of this was condensed with N2-(tert-butoxylcarbonyl)-N6-(benzyloxycarbonyl)-L-lysine in THF contg. Et3N and ClCO2Et and the product selectively deprotected to give N-(N6-benzyloxycarbonyl-L-lysyl)-4-(2-bromobenzyloxycarbonyloxy)-L-phenylalanine 4-acetylanilide-HCl, which was N-acylated with p-MeC6H4COCl and the product treated with 30% aq. HBr to give I [X = p-MeC6H4CO, COY = p-COMe, (OZ)n = p-OCO2CH2C6H4Br-o].HBr. This had an IC50 of 19 .mu.M against fibrin.
IT **120648-33-1P 120672-50-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of protease inhibitors)
RN 120648-33-1 CAPLUS
CN L-Tyrosinamide, N2-(4-methylbenzoyl)-N6-[(phenylmethoxy)carbonyl]-L-lysyl-N-(4-benzoylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



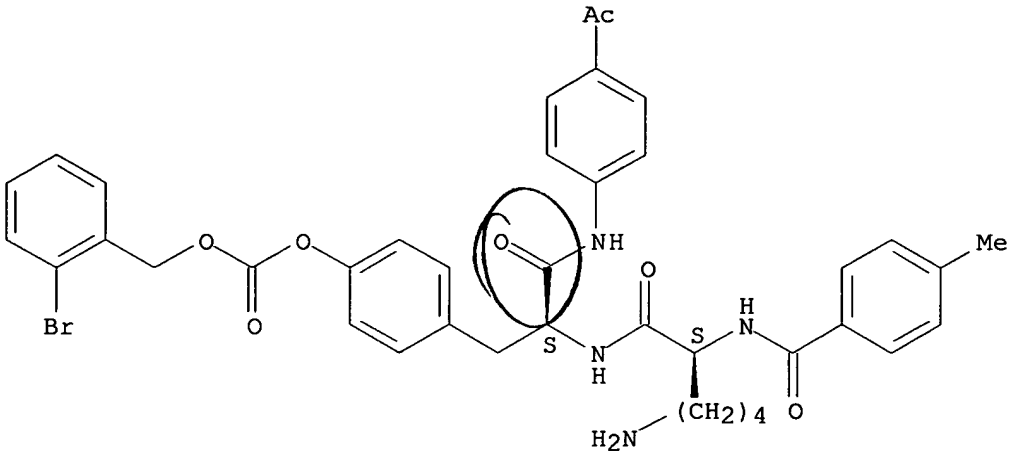
RN 120672-50-6 CAPLUS
CN L-Tyrosinamide, N2-(4-methylbenzoyl)-N6-[(phenylmethoxy)carbonyl]-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **120648-17-1P 120648-18-2P 120648-21-7P**
120648-23-9P 120648-24-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as protease inhibitor)
RN 120648-17-1 CAPLUS
CN L-Tyrosinamide, N2-(4-methylbenzoyl)-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)

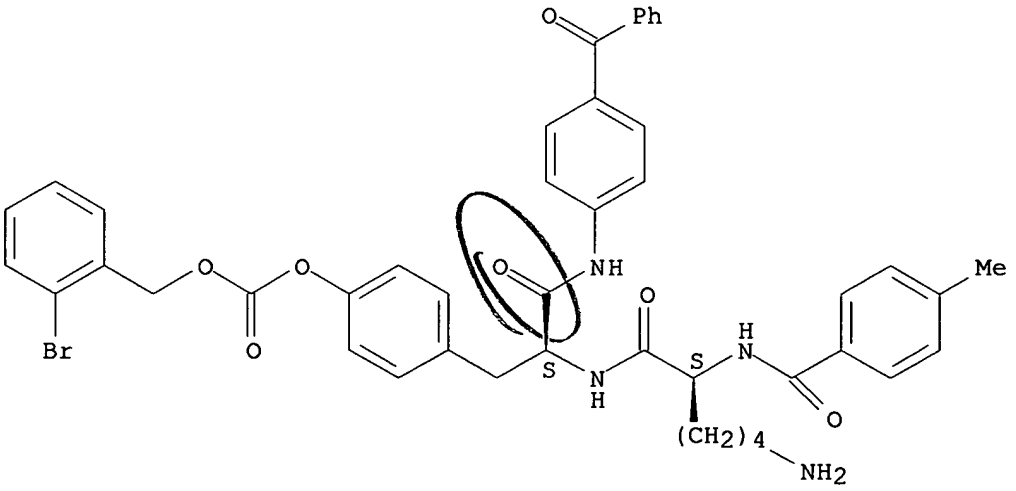
Absolute stereochemistry.



● HBr

RN 120648-18-2 CAPLUS
CN L-Tyrosinamide, N2-(4-methylbenzoyl)-L-lysyl-N-(4-benzoylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)

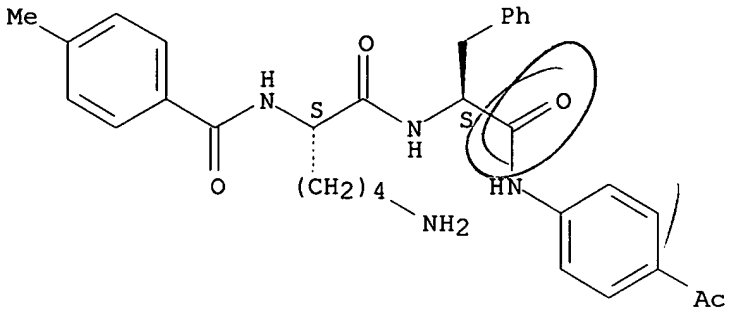
Absolute stereochemistry.



● HBr

RN 120648-21-7 CAPLUS
CN L-Phenylalaninamide, N2-(4-methylbenzoyl)-L-lysyl-N-(4-acetylphenyl)-, monohydrobromide (9CI) (CA INDEX NAME)

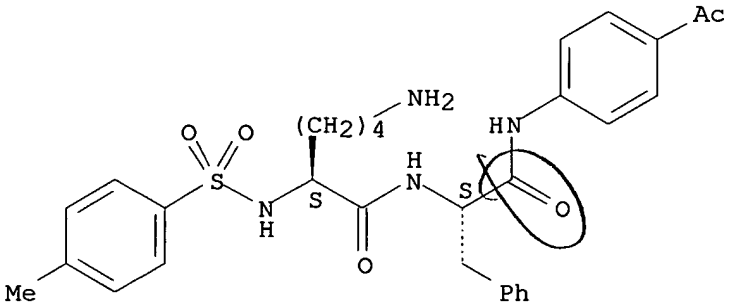
Absolute stereochemistry.



● HBr

RN 120648-23-9 CAPLUS
CN L-Phenylalaninamide, N2-[(4-methylphenyl)sulfonyl]-L-lysyl-N-(4-acetylphenyl)-, monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

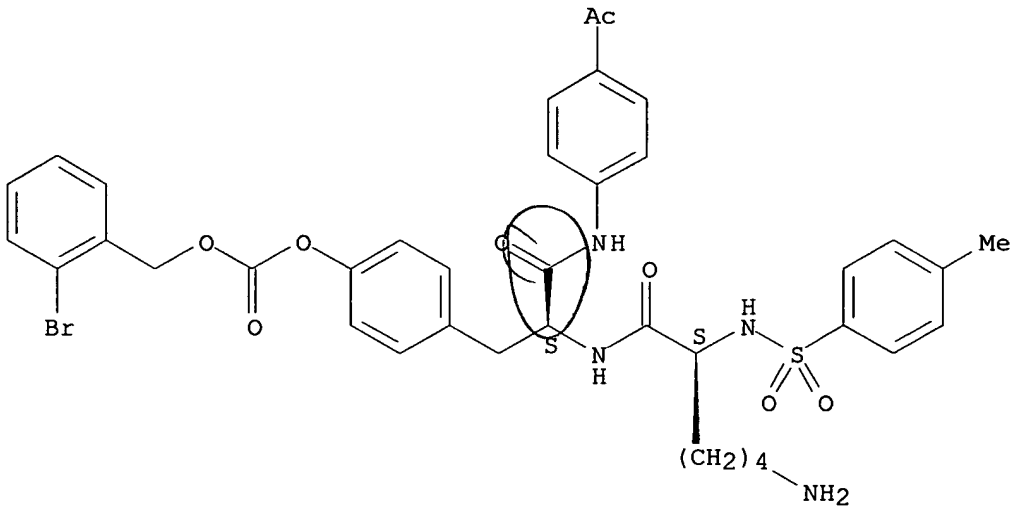


● HBr

RN 120648-24-0 CAPLUS
CN L-Tyrosinamide, N2-[(4-methylphenyl)sulfonyl]-L-lysyl-N-(4-acetylphenyl)-, (2-bromophenyl)methyl carbonate (ester), monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

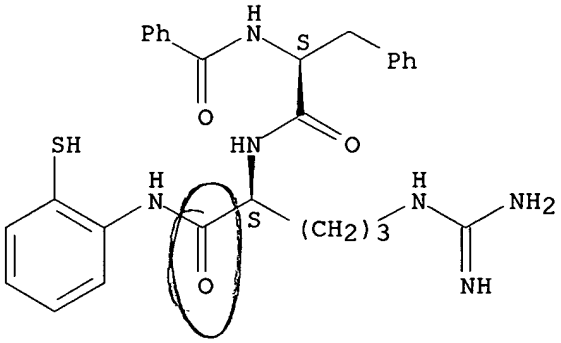


PAGE 2-A

● HBr

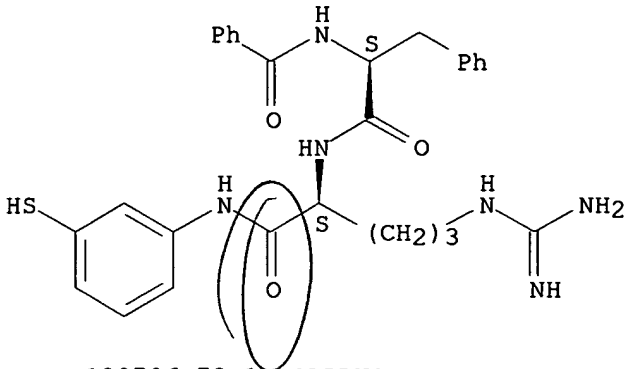
L27 ANSWER 49 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1989:208448 CAPLUS
DN 110:208448
TI Inhibition of Serratia 56K protease by peptidyl mercaptoanilides
AU Nishino, Norikazu; Shimizu, Wataru; Fujimoto, Tsutomu; Maeda, Hiroshi
CS Dep. Appl. Chem., Kyushu Inst. Technol., Kitakyushu, 804, Japan
SO Peptide Chemistry (1989), Volume Date 1988, 26th, 21-4
CODEN: PECHDP; ISSN: 0388-3698
DT Journal
LA English
AB Features of the active site of the 56-kilodalton (56 K) proteinase of S. marcescens were examd. using a no. of peptidyl mercaptoanilide derivs. Enzyme inhibition was related to inhibitor structure, with dependence on peptide chain length (dipeptide required), position of the SH group on the anilide moiety, and deriv. state of the SH group on the anilide moiety (alkylation did not destroy inhibitory activity but affected binding). Ligation of the active site Zn by sulfide was essential for inhibition. A model for inhibitor interaction with the active site is given.
IT **120706-69-6 120706-71-0 120706-72-1**
120706-73-2 120706-74-3 120706-75-4
120706-76-5 120706-77-6 120706-78-7
120706-79-8
RL: BIOL (Biological study)
(proteinase of Serratia marcescens inhibition by, enzyme active site structure in relation to)
RN 120706-69-6 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(2-mercaptophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



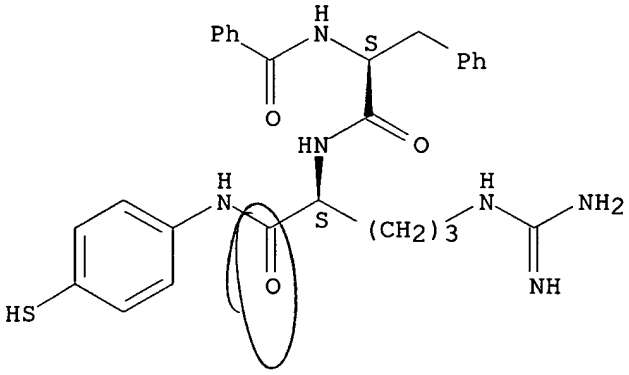
RN 120706-71-0 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(3-mercaptophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



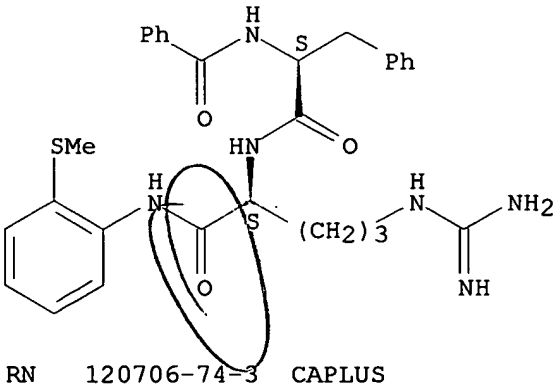
RN 120706-72-1 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-mercaptophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



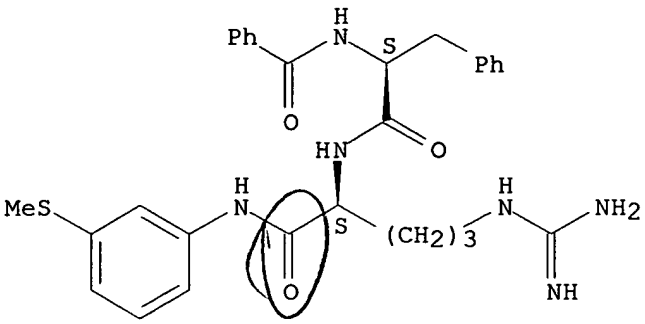
RN 120706-73-2 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[2-(methylthio)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



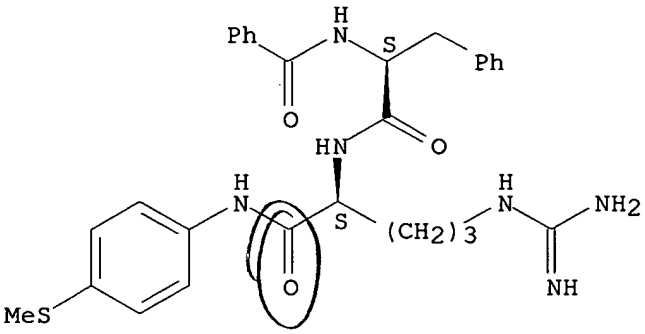
RN 120706-74-3 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[3-(methylthio)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



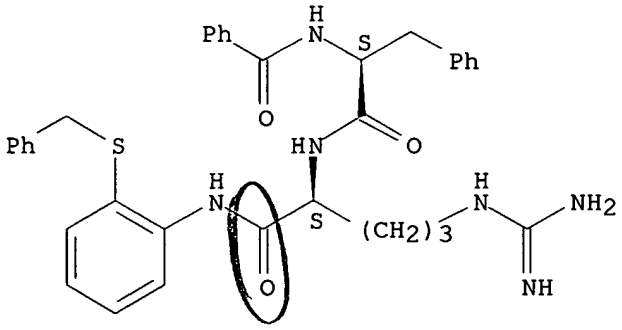
RN 120706-75-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[4-(methylthio)phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



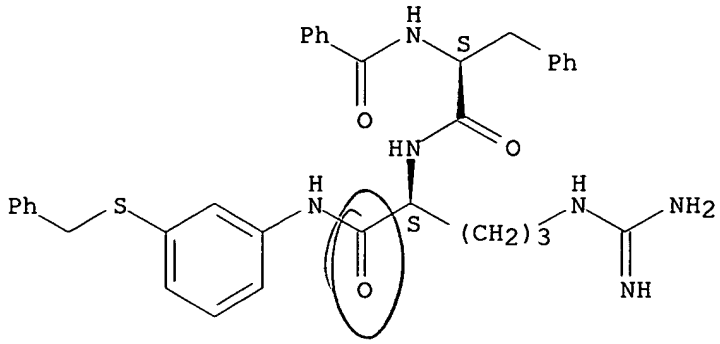
RN 120706-76-5 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[2-[(phenylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



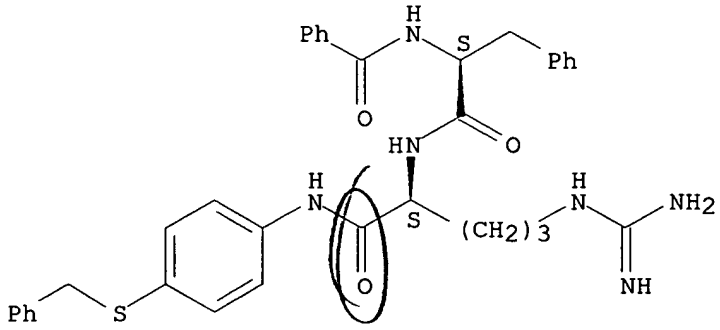
RN 120706-77-6 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[3-[(phenylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



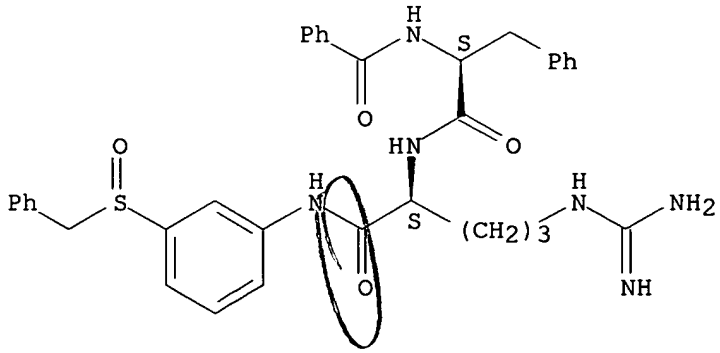
RN 120706-78-7 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[4-[(phenylmethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



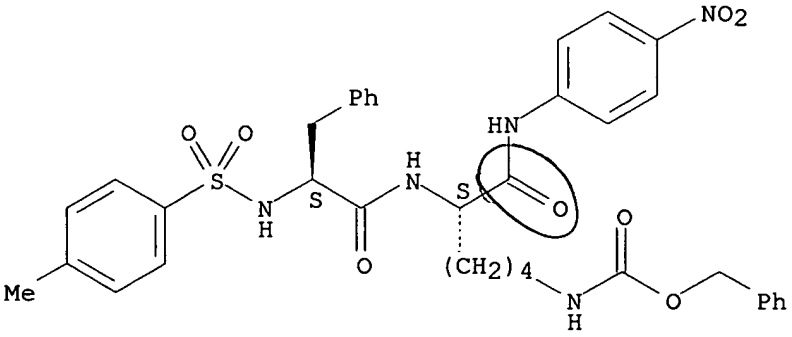
RN 120706-79-8 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-[3-[(phenylmethyl)sulfinyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



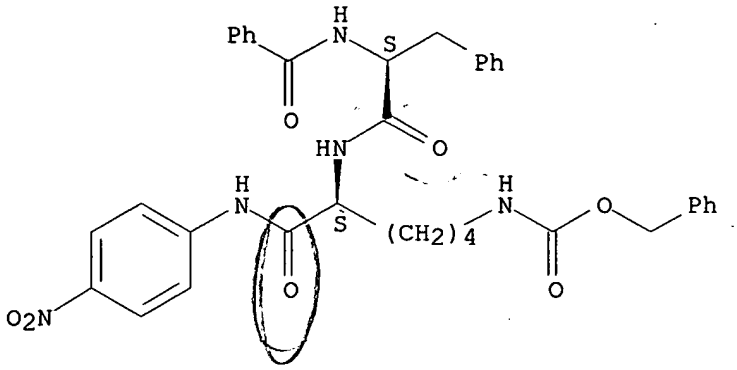
L27 ANSWER 50 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1988:506905 CAPLUS
DN 109:106905
TI Synthesis of active center-directed peptide inhibitors of plasmin
AU Okada, Yoshio; Tsuda, Yuko; Teno, Naoki; Wanaka, Keiko; Bohgaki, Miyako; Hijikata-Okunomiya, Akiko; Naito, Taketoshi; Okamoto, Shosuke
CS Fac. Pharm. Sci., Kobe-Gakuin Univ., Kobe, 673, Japan
SO Chemical & Pharmaceutical Bulletin (1988), 36(4), 1289-97
CODEN: CPBTAL; ISSN: 0009-2363
DT Journal
LA English
OS CASREACT 109:106905
AB Active center-directed peptide inhibitors of plasmin were designed based on the structure of specific substrates of plasmin and synthesized by a conventional soln. method. Their effects on plasmin were examd. and the structure-activity relation was studied. D-Ile-Phe-Lys-BZA (4-benzoylanilide) inhibited plasmin activities toward S-2251 and fibrin (IC50: 0.069 mM and 0.18 mM resp.) but D-Ile-Phe-Lys-BPP (4-benzylpiperidine amide) was not inhibitory. However D-Ile-Phe-Lys-BZA was cleaved by plasmin to release benzoylaniline, indicating that this type of peptide inhibitor is not stable to plasmin. Tos-Lys-pNA was not cleaved by plasmin and inhibited plasmin activity toward not only fibrin but also small peptide substrates and fibrinogen by blocking the active center of plasmin with some selectivity. To obtain potent and stable inhibitors of plasmin, it is recommended to design them with ref. to the structures of Tos-Lys-pNA and the specific substrate D-Ile-Phe-Lys-pNA.
IT **116194-09-3P 116194-11-7P 116194-24-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deprotection of)
RN 116194-09-3 CAPLUS
CN L-Lysinamide, N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-(4-nitrophenyl)-N6-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



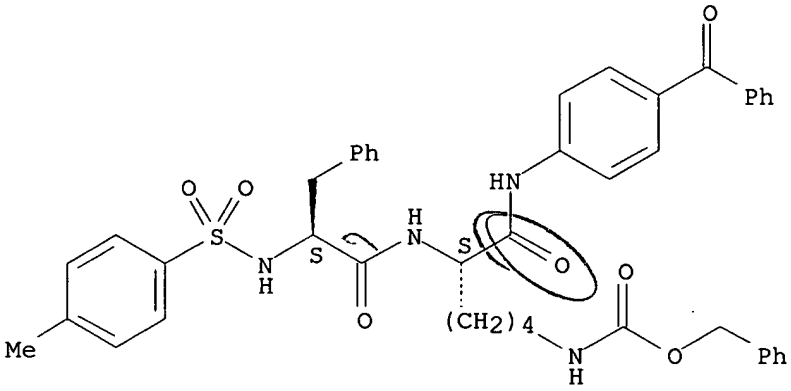
RN 116194-11-7 CAPLUS
CN L-Lysinamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)-N6-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



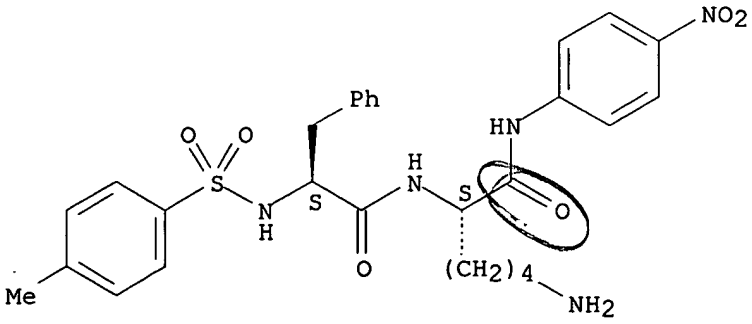
RN 116194-24-2 CAPLUS
CN L-Lysinamide, N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-(4-benzoylphenyl)-N6-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



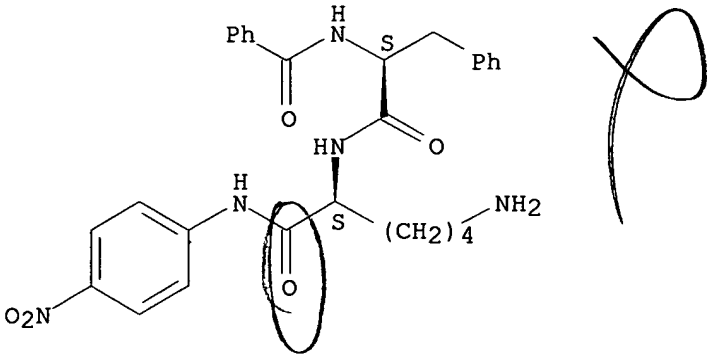
IT **116193-97-6P 116193-99-8P 116194-03-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and plasmin inhibiting activity of)
RN 116193-97-6 CAPLUS
CN L-Lysinamide, N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



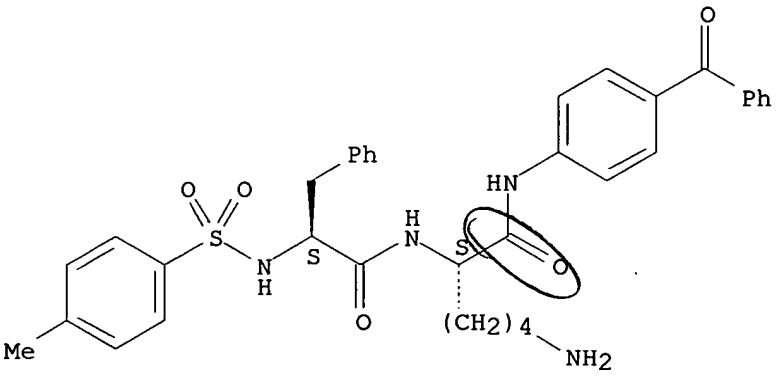
RN 116193-99-8 CAPLUS
CN L-Lysinamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



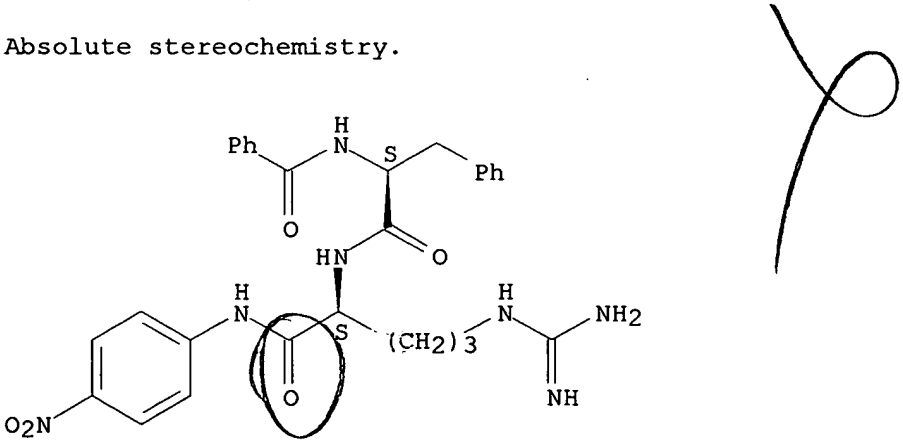
RN 116194-03-7 CAPLUS
CN L-Lysinamide, N-[(4-methylphenyl)sulfonyl]-L-phenylalanyl-N-(4-benzoylphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

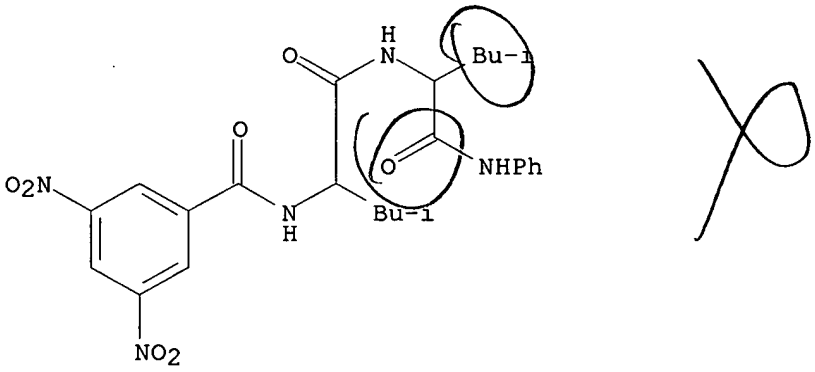


L27 ANSWER 51 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1988:488687 CAPLUS
DN 109:88687
TI Horse urinary kallikrein. II. Effect of subsite interactions on its catalytic activity
AU Araujo-Viel, Mariana S.; Juliano, Maria A.; Oliveira, Laerte; Prado, Eline S.
CS Dep. Bioquim. Biofis., Esc. Paulista de Med., Sao Paulo, 04034, Brazil
SO Biological Chemistry Hoppe-Seyler (1988), 369(5), 397-401
CODEN: BCHSEI; ISSN: 0177-3593
DT Journal
LA English
AB The effect of secondary subsite interactions on the catalytic efficiency of horse urinary kallikrein was studied using as substrates oligopeptides and peptidyl-4-nitroanilides with L-arginine (Arg) at P1. The known secondary specificity of tissue kallikreins for hydrophobic residues at P2 was also demonstrated for horse urinary kallikrein and a higher preference of this enzyme for L-phenylalanine (Phe) over L-leucine (Leu) at P2 was evident. Interaction of enzyme subsites S3 with D-proline (Pro) and D-Phe enhanced the catalytic efficiency but tripeptidyl-4-nitroanilides with acetyl-D-Pro, L-Pro and acetyl-L-Pro at P3 were no better substrates than acetyldipeptidyl-4-nitroanilides. The importance of the leaving group for the catalysis was proved by higher kcat/Km (where kcat is the catalytic rate const.) values for the peptides in relation to peptidyl-4-nitroanilides contg. a common acyl chain. The low kcat value for the peptide with L-Pro at P2' stresses the importance of a H bond between P2' amide and the carbonyl group at S2'. One L-Arg residue at the leaving group, specially at the P2' position, decreases the value of the apparent Km. This effect of side-chain interactions with S2' is impaired by a 2nd L-Arg at P1'.
IT **103418-68-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with kallikrein of horse urine, kinetics of)
RN 103418-68-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

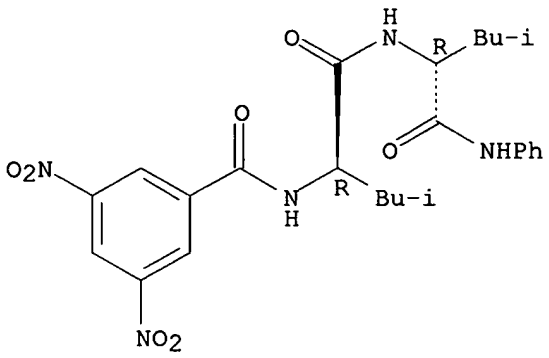


L27 ANSWER 52 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1988:179282 CAPLUS
DN 108:179282
TI Applications for racemic versions of chiral stationary phases
AU Pirkle, William H.; Daeppen, Richard; Reno, Daniel S.
CS Sch. Chem. Sci., Univ. Illinois, Urbana, IL, 61801, USA
SO Journal of Chromatography (1987), 407, 211-16
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB Liq. chromatog. columns packed with the racemic version of a chiral stationary phase may be used in series with the chiral stationary phase column to afford greater peak dispersion for stereoisomeric mixts. than that obtainable with the chiral column alone. The similarity of the mobile phase requirements of a chiral phase and its racemic analog makes the tandem arrangement possible. The capacity ratios noted for enantiomers on a chiral column are contrasted with that noted on the racemic analog.
IT **113339-87-0**
RL: ANST (Analytical study); PROC (Process)
(resoln. of, by liq. chromatog. on racemic and nonracemic stationary phases in series)
RN 113339-87-0 CAPLUS
CN Leucinamide, N-(3,5-dinitrobenzoyl)leucyl-N-phenyl- (9CI) (CA INDEX NAME)



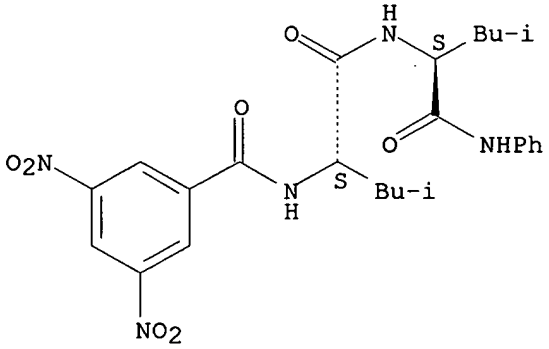
IT **113339-80-3 113339-81-4 113339-84-7**
113382-75-5
RL: ANST (Analytical study); PROC (Process)
(sepn. of, from enantiomers by liq. chromatog. on chiral and chiral racemic stationary phases in series)
RN 113339-80-3 CAPLUS
CN D-Leucinamide, N-(3,5-dinitrobenzoyl)-D-leucyl-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



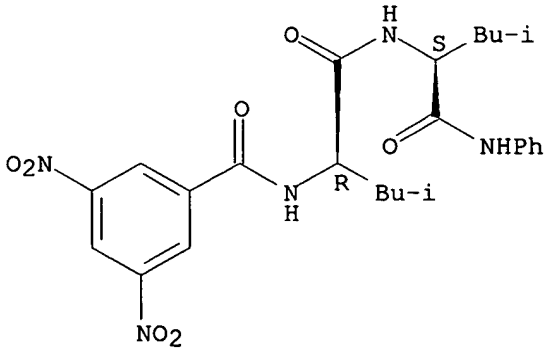
RN 113339-81-4 CAPLUS
CN L-Leucinamide, N-(3,5-dinitrobenzoyl)-L-leucyl-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



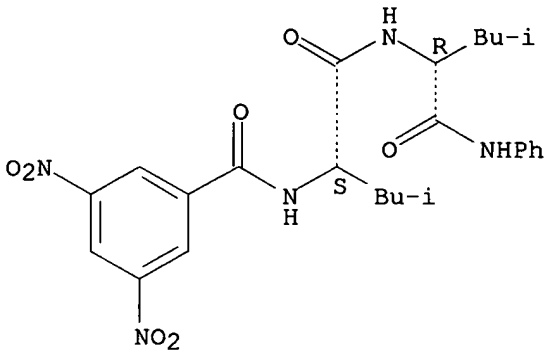
RN 113339-84-7 CAPLUS
CN L-Leucinamide, N-(3,5-dinitrobenzoyl)-D-leucyl-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



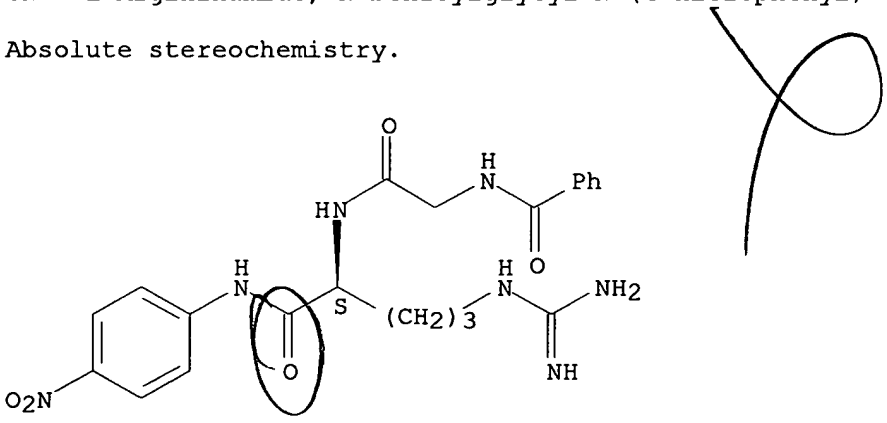
RN 113382-75-5 CAPLUS
CN D-Leucinamide, N-(3,5-dinitrobenzoyl)-L-leucyl-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



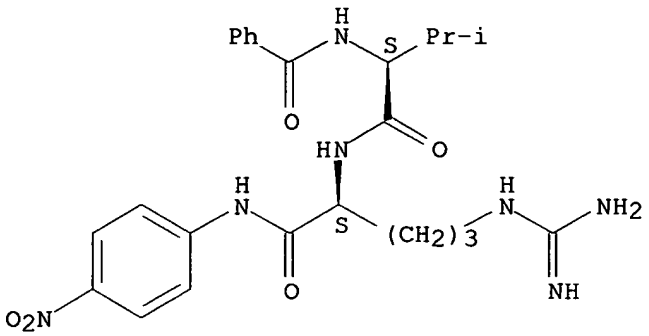
L27 ANSWER 53 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1987:532277 CAPLUS
DN 107:132277
TI The complement component C.hivin.1s catalyzed hydrolysis of peptide 4-nitroanilide substrates
AU Keogh, Shelley J.; Harding, David R. K.; Hardman, Michael J.
CS Dep. Chem. Biochem., Massey Univ., Palmerston North, N. Z.
SO Biochimica et Biophysica Acta (1987), 913(1), 39-44
CODEN: BBACAQ; ISSN: 0006-3002
DT Journal
LA English
AB The kinetic parameter kcat/Km was detd. for the hydrolysis of peptide 4-nitroanilides, catalyzed by complement component C.hivin.1s. Substrates based on the C-terminal sequence of human C4a (Leu-Gln-Arg) were synthesized. Replacement of the glutamine residue by glycine or serine increased kcat/Km. Substitution of valine for the leucine residue increased kcat/Km, while substitution of glycine or lysine for the leucine residue decreased kcat/Km slightly. D-Val-Ser-Arg 4-nitroanilide is the most reactive substrate towards C.hivin.1s, so far. These results are discussed in relation to the amino acid sequences near the bonds cleaved by C.hivin.1s in C4, C2, and C.hivin.1 inhibitor.
IT **103418-67-3P 110325-45-6P 110325-46-7P**
RL: PREP (Preparation)
(prepn. and hydrolysis by complement C1 components)
RN 103418-67-3 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



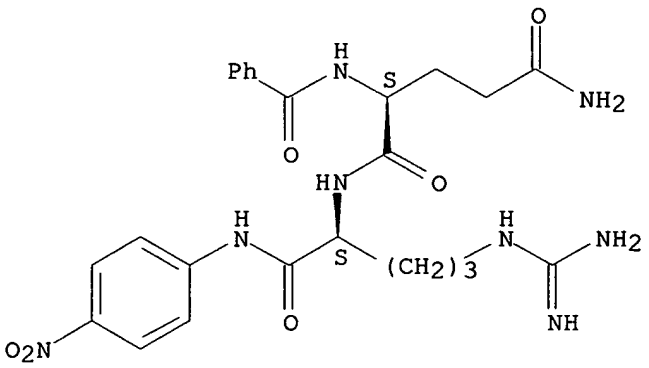
RN 110325-45-6 CAPLUS
CN L-Argininamide, N-benzoyl-L-valyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



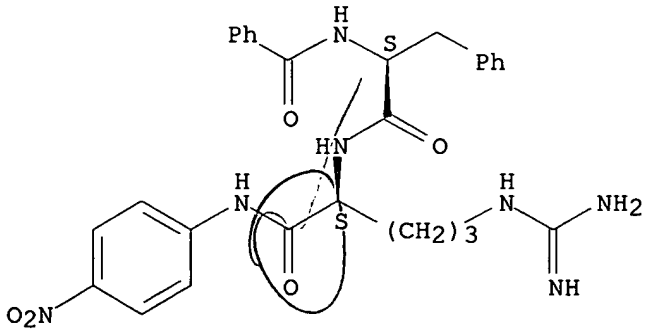
RN 110325-46-7 CAPLUS
CN L-Argininamide, N2-benzoyl-L-glutaminyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



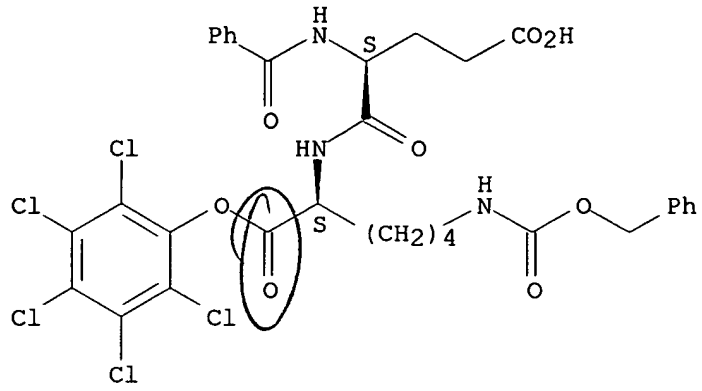
L27 ANSWER 54 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1987:473250 CAPLUS
DN 107:73250
TI Substrate activation of porcine pancreatic kallikrein by N.alpha. derivatives of arginine 4-nitroanilides
AU Oliveira, Laerte; Araujo-Viel, Mariana S.; Juliano, Luiz; Prado, Eline S.
CS Dep. Biochem., Esc. Paul. Med., Sao Paulo, Brazil
SO Biochemistry (1987), 26(16), 5032-5
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB Hydrolysis of several N.alpha.-substituted L-arginine 4-nitroanilides with porcine pancreatic kallikrein was studied under different conditions of pH, temp., and salt concn. At high substrate concns. a deviation from Michaelis-Menten kinetics was obsd. with a significant increase in the hydrolysis rates of almost all substrates. Kinetic data were analyzed on the assumption that porcine pancreatic kallikrein presents an addnl. binding site with lower affinity for the substrate. Binding to this auxiliary site gives rise to a modulated enzyme species which can hydrolyze an addnl. mol. of the substrate through a 2nd catalytic pathway. The values of both Michaelis-Menten and catalytic rate consts. were higher for the modulated species than for the free enzyme, suggesting a mechanism of enzyme activation by substrate. Kinetic data indicated similar substrate requirements for binding at the primary and auxiliary sites of the enzyme. Tris(hydroxymethyl)aminomethane hydrochloride and NaCl altered the kinetic parameters of the hydrolysis of N.alpha.-acetyl-L-Phe-L-Arg 4-nitroanilide by porcine pancreatic kallikrein but not the enzyme activation pattern (ratio of the catalytic consts. for the activated and the free enzyme forms). Similar observations were made when the hydrolysis of D-Val-L-Leu-L-Arg 4-nitroanilide was studied under different pH and temp. conditions.
IT **103418-68-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with kallikrein of pancreas, kinetics of, substrate activation in relation to)
RN 103418-68-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



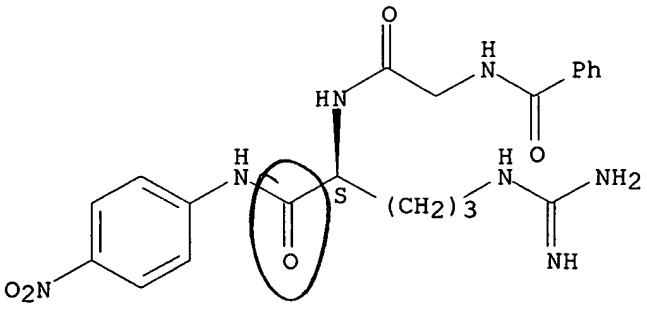
L27 ANSWER 55 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1987:194363 CAPLUS
DN 106:194363
TI Human complement proteins D, C2, and B. Active site mapping with peptide thioester substrates
AU Kam, Chih Min; McRae, Brian J.; Harper, J. Wade; Niemann, Marilyn A.; Volanakis, John E.; Powers, James C.
CS Sch. Chem., Georgia Inst. Technol., Atlanta, GA, 30332, USA
SO Journal of Biological Chemistry (1987), 262(8), 3444-51
CODEN: JBCHA3; ISSN: 0021-9258
DT Journal
LA English
AB The specificity and reactivity of complement serine proteases D, B, Bb, C2, and C2a were detd. using a series of peptide thioester substrates. The rates of thioester hydrolysis were measured using assay mixts. contg. the thiol reagent 4,4'-dithiodipyridine at pH 7.5. Each substrate contained a P1 arginine residue, and the effect of various groups and amino acids in the P2, P3, and P5 positions was detd. using kcat/Km values to compare reactivities. Among peptide thioesters corresponding to the activation site sequence in B, dipeptide thioesters contg. a P2 lysine residue were the best substrates for D. Extending the chain to include a P3 or P4 amino acid resulted in loss of activity, and neither the tripeptide nor the tetrapeptide contg. the cleavage sequence of B was hydrolyzed. Overall, D cleaved fewer substrates and was 2-3 orders of magnitude less reactive than .hivin.C1s against some thioester substrates. C2 and fragment C2a had comparable reactivities and hydrolyzed peptides contg. Leu-Ala-Arg and Leu-Gly-Arg, which have the same sequence as the cleavage sites of C3 and C5, resp. The best substrates for C2 and C2a were Z-Gly-Leu-Ala-Arg-SBzl and Z-Leu-Gly-Leu-Ala-Arg-SBzl, resp., where Bzl is benzyl. B was the least reactive among these complement enzymes. The best substrate for B was Z-Lys-Arg-SBzl with a kcat/Km value of 1370 M-1 s-1. The catalytic fragment of B, Bb, had higher activity toward these peptide thioester substrates. The best substrate for Bb was Z-Gly-Leu-Ala-Arg-SBzl with kcat/Km similar to C2a and 10 times higher than the value for B. Both C2a and Bb were considerably more reactive against C3-like than C5-like substrates. Bovine trypsin hydrolyzed thioester substrates with kcat/Km approx. 103 higher than the complement enzymes. These thioester substrates for D, B, and C2 should be quite useful in kinetic and active site studies of the purified enzymes.
IT **108113-20-8P**
RL: PREP (Preparation)
(prepn. of and reaction with arginine thioester)
RN 108113-20-8 CAPLUS
CN L-Lysine, N2-(N-benzoyl-L-.alpha.-glutamyl)-N6-[(phenylmethoxy)carbonyl]-, 1-(pentachlorophenyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.


Ph
H
N
S
CO2H
O
HN
O
Cl
Cl
O
S
(CH2)4
H
N
O
Ph
O
O
Cl
Cl
Cl

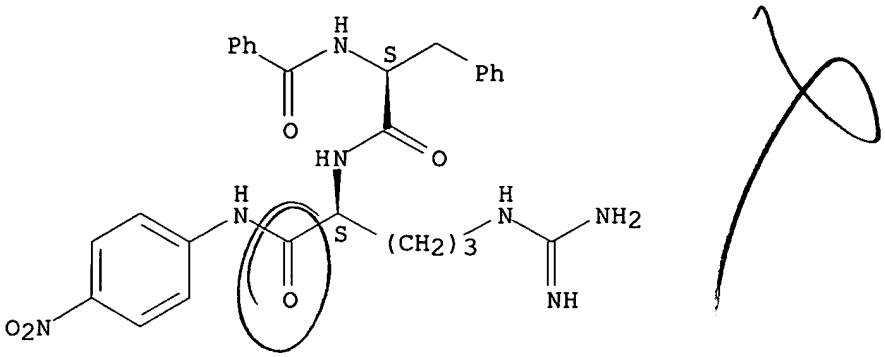
L27 ANSWER 56 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1986:605278 CAPLUS
DN 105:205278
TI Synthesis and kinetic parameters of hydrolysis by trypsin of some acyl-arginyl-p-nitroanilides and peptides containing arginyl-p-nitroanilide
AU Juliano, M. A.; Juliano, L.
CS Dep. Biofis., Esc. Paul. Med., Sao Paulo, 04034, Brazil
SO Brazilian Journal of Medical and Biological Research (1985), 18(4), 435-45
CODEN: BJMRDK; ISSN: 0100-879X
DT Journal
LA English
AB Four acyl-arginyl-p-nitroanilides, 9 acetyl-(or benzoyl)-aminoacyl-arginyl-p-nitroanilides and 12 acyl-(or free .alpha.-amino-)dipeptidyl-arginyl-p-nitroanilides were synthesized, and the kinetic parameters for tryptic hydrolysis of these substrates were detd. in 100 mM Tris-HCl buffer, pH 8.0, contg. 10 mM CaCl2 at 37.degree.. Among the acyl-arginyl-p-nitroanilides, octanoyl-Arg-pNA (where pNA=p-nitroanilide and Arg = arginine) was hydrolyzed 4-fold more rapidly by trypsin than the commonly used substrate benzoyl-Arg-pNa. The best trypsin substrates contain proline and noreleucine at subsite P2, indicating that unbranched aliph. side chain folded as the .beta., .gamma., and .delta. methylenes are in proline provides the most favorable conditions for S2P2 interaction. Extending the length of the substrates from di- to tripeptidyl-pNA did not have a large influence on the kinetic parameters. However, phenylalanine (Phe) at the P3 position had a clear favorable effect, in contrast to proline, which is unfavorable only when the group is present at P4. The series Ac-Phe (or D-Phe)-Gly-Arg-pNA and Phe (or D-Phe)-Gly-Arg-pNA were studied. The benzyl side chain of D-Phe has a more favorable interaction at S3 than Phe (Phe = phenylalanine). A P4-CO...HN-S4 H bond is proposed to stabilize P3/S3 interaction when an acetyl group is present on the .alpha.-amino group of the Phe residue, and the reverse would be expected to occur for the corresponding D-epimer.
IT **103418-67-3P 103418-68-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and trypsin reaction kinetics with)
RN 103418-67-3 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

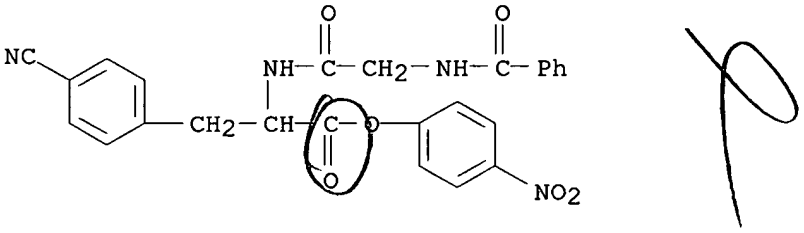


RN 103418-68-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

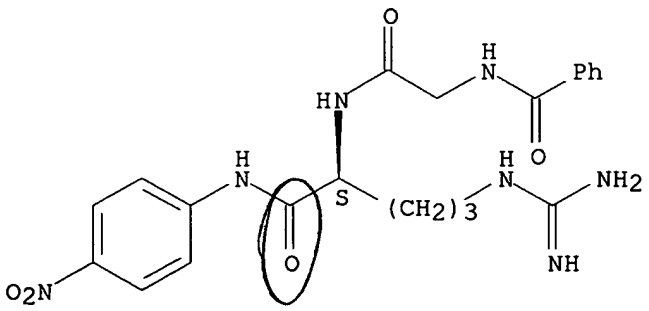


L27 ANSWER 57 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1986:497888 CAPLUS
DN 105:97888
TI Synthesis of N.alpha.-(benzoylglycyl)- and N.alpha.-(benzyloxycarbonylglycyl)-4-amidinophenylalanine as thrombin inhibitors
AU Voigt, B.; Wagner, G.
CS Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.
SO Pharmazie (1985), 40(8), 527-9
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
OS CASREACT 105:97888
AB Dipeptides I (R = Bz, PhCH2O2C) were condensed with HNR1R2 (NR1R2 = piperidino, pyrrolidino, morpholino, NBu) to give dipeptide amides II (R, R1, R2 = same), which were treated with H2S to give thioamides III, which were S-methylated with MeI to give thioimidic esters IV, which were treated with NH4OAc to give title compds. V. V can be used as thrombin inhibitors; V (R = PhCH2O2C, NR1R2 = piperidino) was the most effective inhibitor.
IT **103879-80-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and amidation of)
RN 103879-80-7 CAPLUS
CN Phenylalanine, N-(N-benzoylglycyl)-4-cyano-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



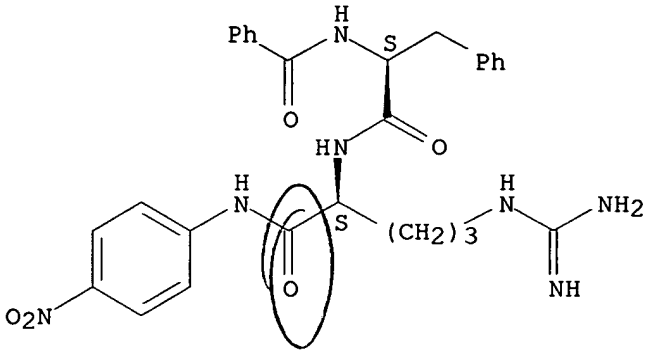
L27 ANSWER 58 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1986:456903 CAPLUS
DN 105:56903
TI Synthesis and kinetic parameters of hydrolysis by trypsin of some acyl-arginyl-p-nitroanilides and peptides containing arginyl-p-nitroanilide
AU Juliano, M. A.; Juliano, L.
CS Dep. Biofis., Esc. Paulista Med., Sao Paulo, 04034, Brazil
SO Brazilian Journal of Medical and Biological Research (1985), 18(4), 435-45
CODEN: BJMRDK; ISSN: 0100-879X
DT Journal
LA English
AB Four acylarginine-p-nitroanilides, 9 acetyl- (or benzoyl)aminoacylarginine-p-nitroanilides, and 12 acyl- (or free .alpha.-amino-)dipeptidylarginine-p-nitroanilides were synthesized, and the kinetic parameters for tryptic hydrolysis of these substrates were detd. in 100 mM Tris-HCl buffer, pH 8.0, contg. 10 mM CaCl2 at 37.degree.. Among the acylarginine-p-nitroanilides, octanoylarginine-p-nitroanilide was hydrolyzed 4-fold more rapidly by trypsin than the commonly used substrate, benzoylarginine-p-nitroanilide. The best trypsin substrates contained proline and norleucine at subsite P2, indicating that unbranched aliph. side-chain folded, as the .beta., .gamma., and .delta. methylenes are in proline, provides the most favorable conditions for S2P2 interaction. Extending the length of the substrates from di- to tripeptidyl-p-nitroanilide did not have a large influence on the kinetic parameters. However, phenylalanine at the P3 position had a clearly favorable effect, in contrast to proline, which was unfavorable only when the benzoyl group was present at P4. The series, Ac-Phe-(or D-Phe)-Gly-Arg-p-nitroanilide and Phe-(or D-Phe)-Gly-Arg-p-nitroanilide were studied. The benzyl side-chain of D-phenylalanine had a more favorable interaction at S3 than phenylalanine. A P4-CO...HN-S4 H-bond was proposed to stabilize the P3/S3 interaction when an Ac group was present on the .alpha.-NH2 group of the phenylalanine residue, and the reverse would be expected to occur for the corresponding D-epimer.
IT **103418-67-3P 103418-68-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction kinetics with trypsin)
RN 103418-67-3 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

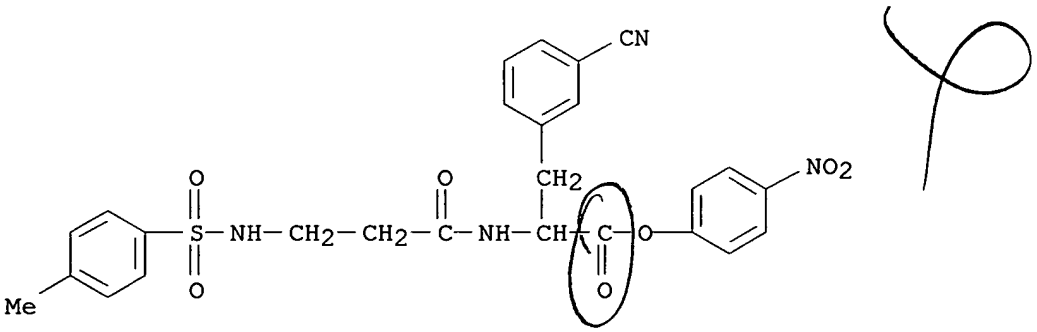


RN 103418-68-4 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

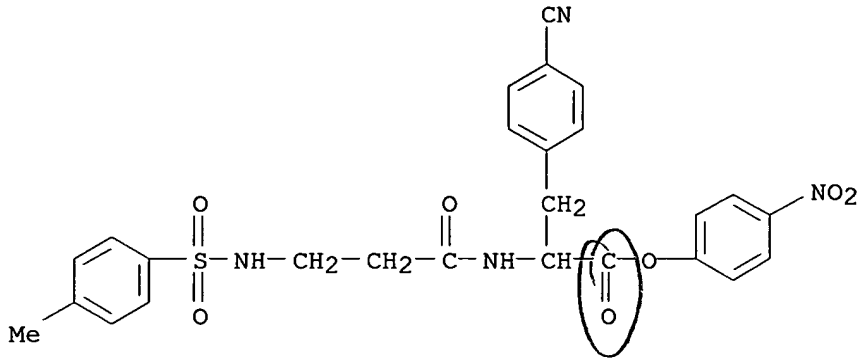
Absolute stereochemistry.



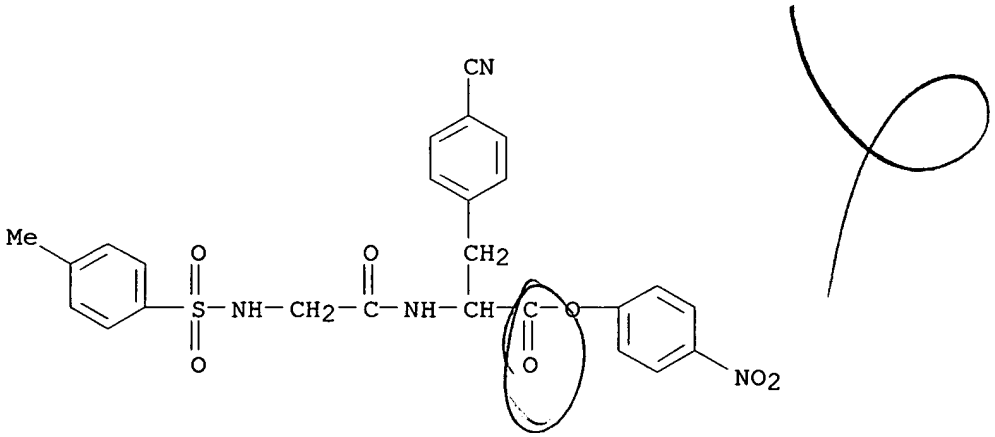
L27 ANSWER 59 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1984:631006 CAPLUS
DN 101:231006
TI Synthesis of N.alpha.-(tosyl-.beta.-alanyl)- and N.alpha.-(tosyl-.epsilon.-aminocapronyl)amidinophenylalaninamides as very effective thrombin inhibitors
AU Wagner, G.; Voigt, B.; Pfeiffer, Christine
CS Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.
SO Pharmazie (1984), 39(5), 315-17
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
AB Title compds. I (Tos = tosyl; NRR1 = piperidino, morpholino, pyrrolidino; position of arom. substitution = 3 or 4) and II (position of arom. substitution = 3 or 4) were prepd. from the corresponding cyanophenylalanines III in several steps. Thus, III was acylated with Tos-.beta.-Ala-Cl to give dipeptides IV (R2 = 3- or 4-CN, R3 = OH), which were esterified with HOC6H4NO2-4 by DCC to give IV (R2 = same, R3 = OC6H4NO2-p), which were amidated with HNRR1 (NRR1 = same) to give IV (R2 = same, R3 = NRR1). The latter were treated with H2S to give IV [R2 = 3- or 4-C(S)NH2, R3 = NRR1], which were treated with MeI to give IV.HI (R2 = 3- or 4-C(:NH)SMe, R3 = NRR1), which were treated with NH4OAc to give I. II were prepd. similarly from III and TosNH(CH2)5COCl. The prolongation of the C-chain of the branchless amino acid decreased the antithrombin activity.
IT **93235-66-6P 93235-67-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and amidation of)
RN 93235-66-6 CAPLUS
CN Phenylalanine, 3-cyano-N-[N-[(4-methylphenyl)sulfonyl]-.beta.-alanyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



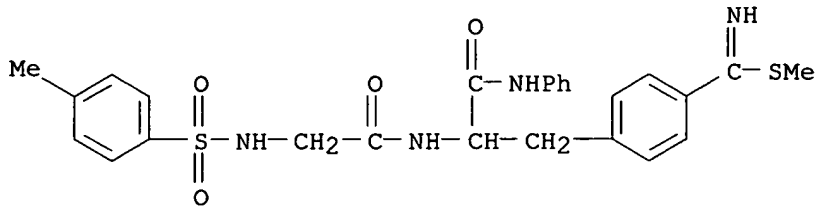
RN 93235-67-7 CAPLUS
CN Phenylalanine, 4-cyano-N-[N-[(4-methylphenyl)sulfonyl]-.beta.-alanyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)


CN
O
O
CH2
NO2
S
NH
CH2
CH2
C
NH
CH
C
O
O
O
Me

L27 ANSWER 60 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1984:611666 CAPLUS
DN 101:211666
TI Synthesis of N.alpha.-(arylsulfonylglycyl)amidinophenylalaninamides as highly active inhibitors of thrombin
AU Wagner, G.; Voigt, B.; Vieweg, H.
CS Sekt. Biowiss., Karl-Marx-Univ. Leipzig, Leipzig, DDR-7010, Ger. Dem. Rep.
SO Pharmazie (1984), 39(4), 226-30
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
AB The title compds. I (R = piperidino, pyrrolidino, BuNH, PhNH, morpholino; R1 = p-tolyl, .alpha.-, .beta.-naphthyl; amidino at 3 or 4), as the HCl or HI salts, were prepd. from purified cyanophenylalanines after introducing the arylsulfonylglycyl group, activating the CO2H group by forming the 4-O2NC6H4 ester, subsequent aminolysis, and conversion of the cyano into an amidino function. Addnl., several esters and an acid with the basic structure of I were prepd. I (R = piperidino, R1 = 2-naphthyl, 4-amidino) had the strongest antithrombin activity with Ki = 6 .times. 10-9 mol/L using S-2238 substrate.
IT **84792-45-0P 92740-67-5P 92771-17-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and aminolysis of)
RN 84792-45-0 CAPLUS
CN Phenylalanine, 4-cyano-N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

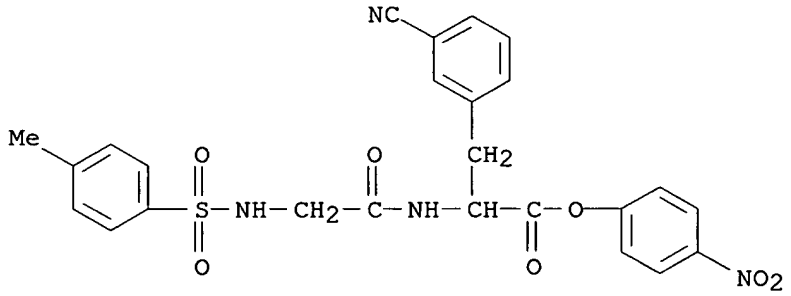


RN 92740-67-5 CAPLUS
CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-[imino(methylthio)methyl]-N-phenyl-, monohydriodide (9CI) (CA INDEX NAME)

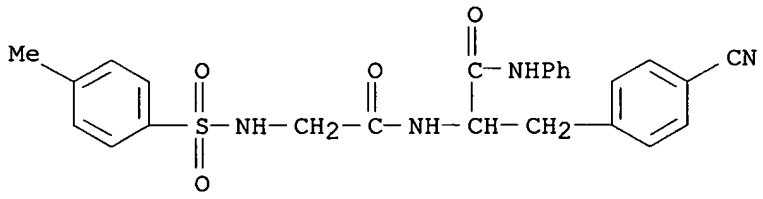


● HI

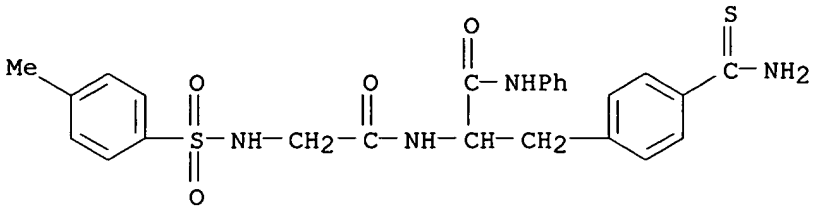
RN 92771-17-0 CAPLUS
CN Phenylalanine, 3-cyano-N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



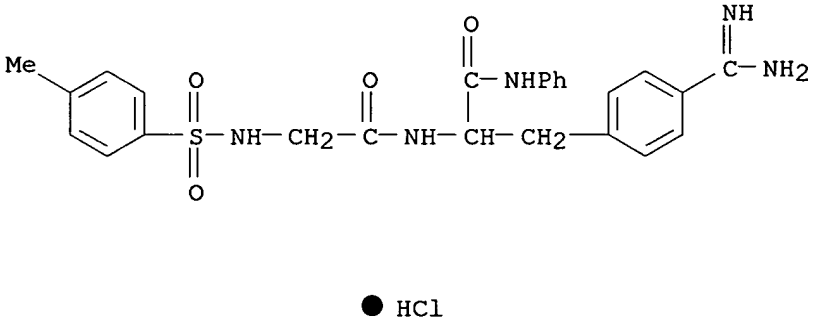
IT **92771-23-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrosulfuration of)
RN 92771-23-8 CAPLUS
CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-cyano-N-phenyl- (9CI) (CA INDEX NAME)



IT **92771-14-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and S-methylation of)
RN 92771-14-7 CAPLUS
CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-(aminothioxomethyl)-N-phenyl- (9CI) (CA INDEX NAME)

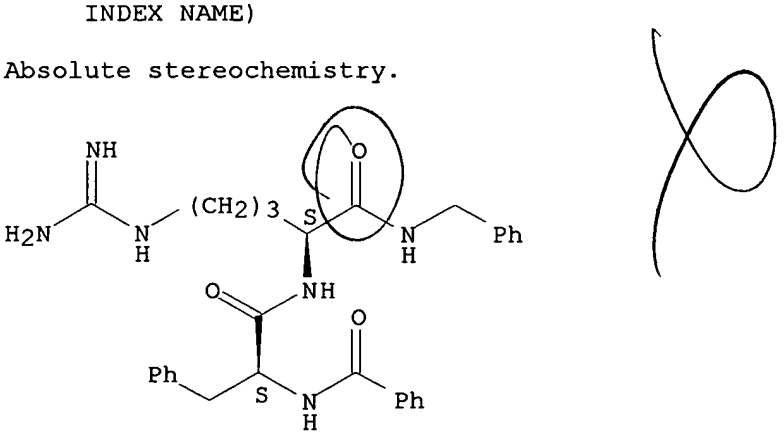


IT **92842-14-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as thrombin inhibitor)
RN 92842-14-3 CAPLUS
CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-(aminoiminomethyl)-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



L27 ANSWER 61 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1983:418458 CAPLUS
DN 99:18458
TI Simple radioassays for human plasma and glandular kallikreins
AU Ryan, James W.; Hernandez, Pedro A.; Chung, Alfred; Valido, Fernando
CS Sch. Med., Univ. Miami, Miami, FL, 33101, USA
SO Advances in Experimental Medicine and Biology (1983), 156A(Kinins-3, Pt. A), 241-9
CODEN: AEMBAP; ISSN: 0065-2598
DT Journal
LA English
AB Various peptide substrates were investigated in developing radiochem. assays for human urinary and plasma kallikrein (I). The optimal substrate (of 12 tested) for urinary I was D-Pro-Phe-Arg-[3H]benzylamide; salts and bovine serum albumin (<0.2 mg/mL) did not influence the reaction. For detn. of plasma I, pyroGlu-Phe-Arg-[3H]benzylamide was the optimal substrate; bovine serum albumin (0.4%) increased the reaction rate .apprx.7-fold. Plasmin hydrolyzed the latter substrate as well, with Kcat/Km 106-fold greater than that for plasma I.
IT **86125-77-1**
RL: BIOL (Biological study)
(in detn. of kallikrein of human urine and plasma)
RN 86125-77-1 CAPLUS
CN L-Argininamide, N-benzoyl-L-phenylalanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

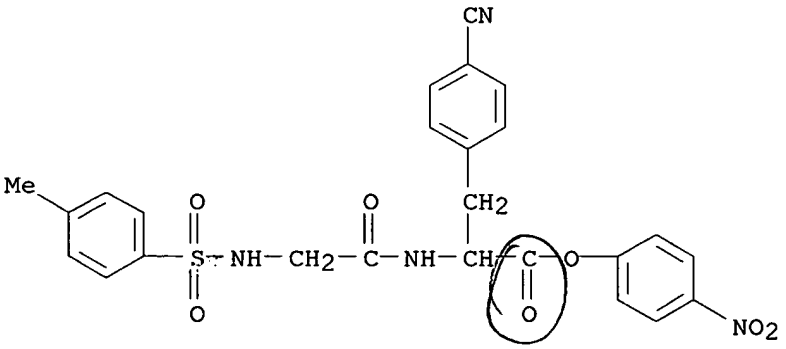
Absolute stereochemistry.



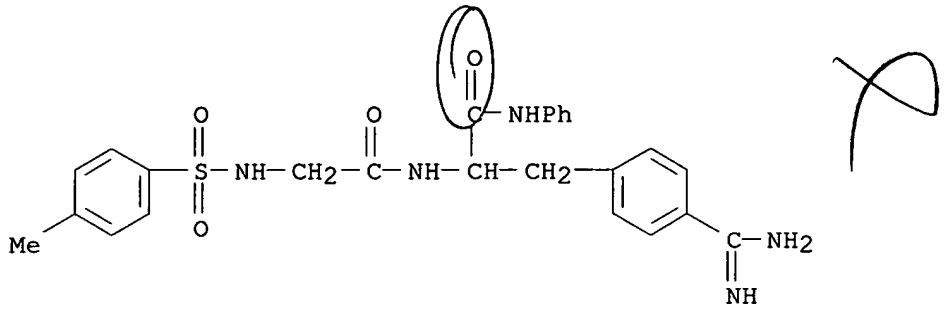
L27 ANSWER 62 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1983:107770 CAPLUS
DN 98:107770
TI N.alpha.-Aryl- or N.alpha.-heteroarylsulfonyl aminoacylated amidinophenylalanine amides
IN Wagner, Guenther; Voigt, Bernd; Vieweg, Helmut; Markwardt, Fritz; Stuerzebecher, Joerg
PA Ger. Dem. Rep.
SO Ger. (East), 17 pp.
CODEN: GEXXA8
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DD 155954	Z	19820721	DD 1981-227387	19810203
DD 155954	B1	19881109		
PRAI DD 1981-227387		19810203		

OS CASREACT 98:107770
AB Title compds. I (R = aryl, heteroaryl; R1 = H, alkyl, aryl, aralkyl; R2 = alkyl, aryl, aralkyl; NR1R2 = heteroaliph. ring; n = 1-5; amidino group at m- or p-position) were prepd. as thrombin inhibitors for use as anticoagulants (no data). Thus, Tos-Gly-Cl (Tos = tosyl) was coupled with 3- and 4-cyanophenylalanine-HCl in 1N NaOH to give peptide II and its p-isomer, which were esterified with HOC6H4NO2-4 by DCC to give the p-nitrophenyl esters, which were treated with piperidine to give piperidides III (R3 = m-CN, p-CN). The latter were treated with H2S to give the thioamides, which were treated with MeI and then with NH4OAc/MeOH to give III [R3 = m-C(:NH)NH2, p-C(:NH)NH2].
IT **84792-45-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with piperidine)
RN 84792-45-0 CAPLUS
CN Phenylalanine, 4-cyano-N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



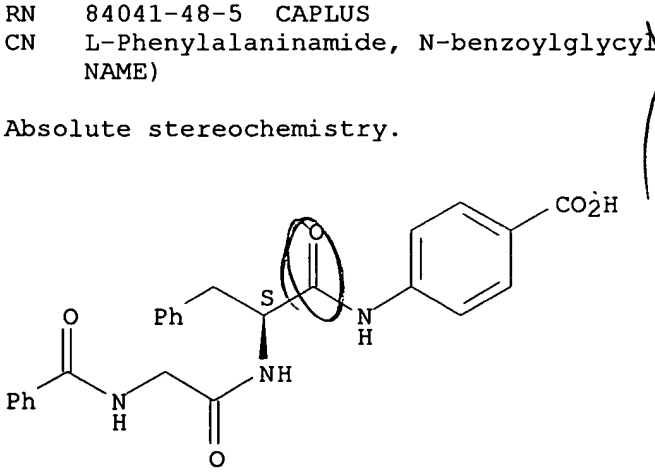
IT **84792-59-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 84792-59-6 CAPLUS
CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-(aminoiminomethyl)-N-phenyl-, monohydriodide (9CI) (CA INDEX NAME)



● HI

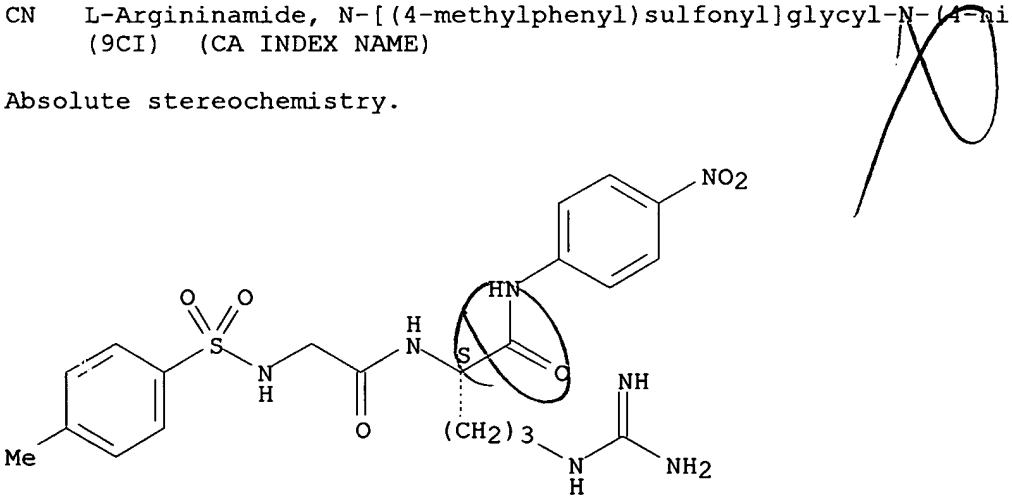
L27 ANSWER 63 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1983:67751 CAPLUS
DN 98:67751
TI Membrane-bound kidney neutral metalloendopeptidase: interaction with synthetic substrates, natural peptides, and inhibitors
AU Almenoff, June; Orlowski, Marian
CS Mt. Sinai Sch. Med., City Univ. New York, NY, 10029, USA
SO Biochemistry (1983), 22(3), 590-9
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB A neutral metalloendopeptidase with thermolysin-like specificity was purified to apparent homogeneity from the particulate fraction of rabbit kidney homogenates. After prepn. of a deoxycholate ext., the enzyme was released from membranes by papain treatment and sepd. from other membrane-bound enzymes including dipeptidyl aminopeptidase IV, aminopeptidase M, and .gamma.-glutamyl transpeptidase by chromatog. on Sephadex G-200, phenyl-Sepharose, and CM-cellulose columns. The isolated enzyme had a mol. wt. of .apprx.95,000 and was inhibited by thiols, metal chelators, phosphoramidon, and thiorphan. It was apparently identical with kidney neutral metalloendopeptidase and similar to bovine pituitary metalloendopeptidase and to an enzyme designated as enkephalinase. Studies with a series of synthetic substrates showed that the enzyme preferentially cleaved bonds in which the amino group was provided by a hydrophobic amino acid residue. Several biol. active peptides, such as methionine- and leucine-enkephalin, dynorphin, bradykinin, and angiotensin I, were degraded by cleavage of the same type of bond. The endopeptidase acted as a dipeptidyl carboxypeptidase on peptides having a hydrophobic residue in the penultimate position. N-[1(RS)-Carboxy-2-phenylethyl] derivs. of phenylalanyl- and alanyl-p-aminobenzoate were synthesized and tested as potential inhibitors. The two diastereomers of N-[1(R,S)-carboxy-2-phenylethyl]phenylalanyl-p-aminobenzoate were sepd. by high-pressure liq. chromatog.; the more potent isomer had a Ki of 2.9 .times. 10-8 M. The inhibitory potency of the alanyl derivs. was lower by almost 2 orders of magnitude. The data indicated that, as with thermolysin, a hydrophobic residue in the P1' position and the carboxylate group complexing with the active-site Zn accounted for the inhibitory action of these derivs.
IT **84041-48-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of and metalloendopeptidase of kidney inhibition by)
RN 84041-48-5 CAPLUS
CN L-Phenylalaninamide, N-benzoylglycyl-N-(4-carboxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 64 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1983:49235 CAPLUS
DN 98:49235
TI Two automated methods for plasma antithrombin III compared, and the clinical significance of the results
AU Prellwitz, Winfried; Schmitt, Karl Friedrich; Machner, Mathias; Schuster, Carl Johannes; Weilemann, Ludwig
CS Dep. Clin. Chem., Univ. Mainz, Mainz, D 6500, Fed. Rep. Ger.
SO Clinical Chemistry (Washington, DC, United States) (1982), 28(11), 2249-53
CODEN: CLCHAU; ISSN: 0009-9147
DT Journal
LA English
AB Antithrombin III (AT III) activity was detd. with 2 different new chromogenic substances [Chromozym-TH (tosyl-Gly-Arg-p-nitroanilide) and .alpha.-N-carbobenzyloxy-L-lysine-thiobenzyl ester] with both a discrete (aca) and a centrifugal analyzer (COBAS BIO). The correlation between the Chromozym-TH/centrifugal analyzer and Du Pont ester/aca methods was good. Precision within and between runs was similar to that for typical enzymic detns. AT III in plasma of healthy men and women ranged 76.6-141.1% (100% = normal). No significant differences ascribable to oral contraceptives were found. AT III activity was decreased in 27% of patients with acute thromboembolic diseases, in 48% of patients the 1st day after abdominal operations without complications, and in 100% of patients with reversible or irreversible shock. In patients receiving continuous therapy with heparin (1500 USP units/h), no decrease in AT III within 96 h of beginning treatment was obsd. Plasma from 14 of 16 patients with disseminated intravascular coagulopathy showed a decrease in AT III of 17-51% of normal before and during heparin therapy. All 16 patients were treated with AT III conc. During such treatment, AT III in plasma must be monitored over short intervals to assure that sufficiently high proportions of AT III (>70% of normal) are reached.
IT **84213-42-3**
RL: BIOL (Biological study)
(in antithrombin III detn., in blood plasma of humans)
RN 84213-42-3 CAPLUS
CN L-Argininamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-(4-nitrophenyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 65 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1982:472781 CAPLUS
DN 97:72781
TI Tumor-resolving and histolytic medicaments and their use
IN Etschenberg, Eugen; Opitz, Wolfgang; Raddatz, Siegfried
PA Troponwerke G.m.b.H. und Co. K.-G., Fed. Rep. Ger.
SO U.S., 26 pp. Cont.-in-part of U.S. Ser. No. 862,896, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

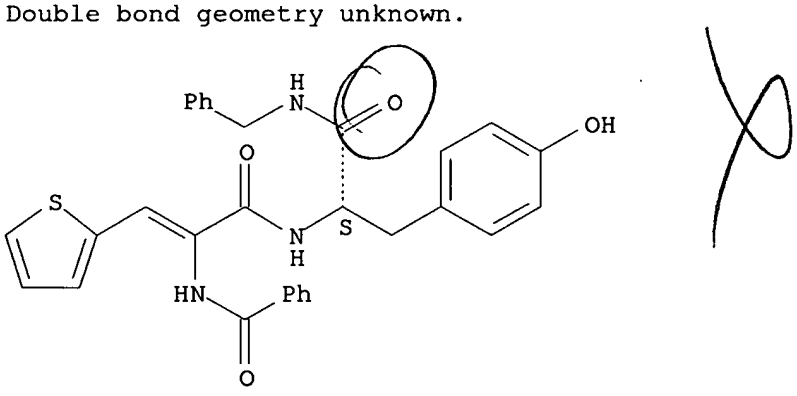
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4310517	A	19820112	US 1979-82450	19791009
	DE 2659154	A1	19780706	DE 1976-2659154	19761228
	DE 2745673	A1	19790412	DE 1977-2745673	19771011
PRAI	DE 1976-2659154		19761228		
	DE 1977-2745673		19771011		
	US 1977-862896		19771221		

AB Dehydropeptides R-(NHCHR1CO)m-NHC(:CR2R3)-CO-(NR4CHR5CO)n-[NHC(:CR6R7)CO]p-(NHCR8R9CO)q-R10 [R = H, alkanoyl, heteroaryl, (un)substituted Bz, naphthyl; R1, R5, R8 = H, alkyl, (un)substituted phenylalkyl; R2, R6, R9 = H, alkyl; R3, R7 = (un)substituted Ph, naphthyl; R4 = H; R4R5 = alkylene; R10 = OH, (un)substituted NHNH2, NH2; m, n, p, q = 0, 1] were prepd. as antitumor agents (no data). Thus, oxazolone I was treated with proline to give 59% AcNHC(:CHPh)CO-Pro-OH.

IT **68763-36-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 68763-36-0 CAPLUS
CN L-Tyrosinamide, N-benzoyl-2,3-didehydro-3-(2-thienyl)alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L27 ANSWER 66 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1982:7087 CAPLUS
DN 96:7087
TI Dehydrooligopeptides and their medicinal use
IN Etschenberg, Eugen; Opitz, Wolfgang; Raddatz, Siegfried
PA Troponwerke G.m.b.H. und Co. K.-G., Fed. Rep. Ger.
SO U.S., 16 pp. Cont.-in-part of U.S. Ser. No. 863,208, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

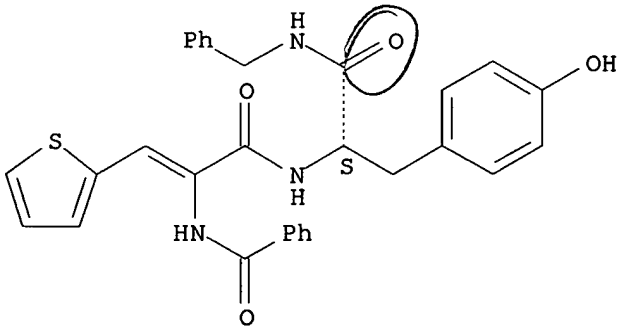
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4276288	A	19810630	US 1979-82451	19791009
	DE 2659114	A1	19780706	DE 1976-2659114	19761228
	DE 2745584	A1	19790419	DE 1977-2745584	19771011
PRAI	DE 1976-2659114		19761228		
	DE 1977-2745584		19771011		
	US 1977-863208		19771222		

AB Dehydropeptides RCONHC(:CR1R2)CO[NHC(:CR3R4)CO]m(NHCHR5CO)nR6 (R = C1-6 alkyl optionally substituted by 1-3 halogen atoms or C1-3 alkoxy; Ph, styryl, or thienyl; R1 = H, C1-4 alkyl; R2 = Ph, naphthyl, C4-6 cycloalkyl, C1-4 alkyl, unsatd. heterocyclic radical optionally substituted by NO2; CR1R2 = cyclopentylidene, cyclohexylidene, cyclopentenylidene, or cyclohexenylidene; R3 = H, Me, Et; R4 = Ph substituted by 1-3 halogen or a 5-7-membered heterocyclic group contg. 1 or 2 N, O, or S atoms; R5 = CH2Ph substituted by 1 or 2 halogen atoms or by OH or NO2; CH2CH2SMe or CH2CO2H; R6 = OH, NH2, C1-10 alkylamino, C1-5 alkoxy, dialkylamino; m and n = 0 or 1) were prepd. as antitumor agents (no data). Thus, oxazolone I was treated with D-proline to give 55% AcNHC(:CHPh)CO-D-Pro-OH.

IT **68763-36-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 68763-36-0 CAPLUS
CN L-Tyrosinamide, N-benzoyl-2,3-didehydro-3-(2-thienyl)alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L27 ANSWER 67 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1981:175538 CAPLUS
DN 94:175538
TI Tumor-resolving and histolytic medicaments comprising dehydrooligopeptides
IN Etschenberg, Eugen; Opitz, Wolfgang; Raddatz, Siegfried
PA Troponwerke G.m.b.H. und Co. K.-G., Fed. Rep. Ger.
SO Brit., 48 pp.
CODEN: BRXXAA
DT Patent
LA English
FAN.CNT 3

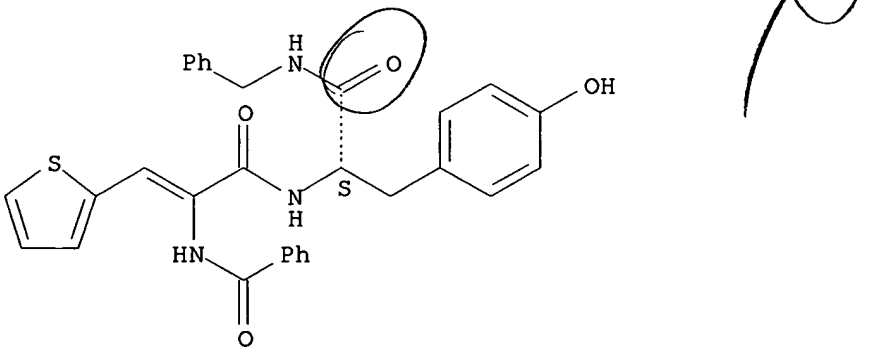
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1570140	A	19800625	GB 1977-53179	19771221
	DE 2659154	A1	19780706	DE 1976-2659154	19761228
	DE 2745673	A1	19790412	DE 1977-2745673	19771011
PRAI	DE 1976-2659154		19761228		
	DE 1977-2745673		19771011		

AB Pharmaceutical compns. contg. 1-90% wt. of dehydrooligopeptides or their salts, prepd. by alk. hydrolysis of the corresponding 2,4-disubstituted 5(4H)oxazolones or by aminolysis of the oxazolones with the alkali metal salts, esters, or amides of amino acids, showed tumor resolving and histolytic activity with low toxicity and good general tolerance when administered at 1-100 mg/kg/day.

IT **68763-36-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for neoplasm inhibiting oligopeptides)

RN 68763-36-0 CAPLUS
CN L-Tyrosinamide, N-benzoyl-2,3-didehydro-3-(2-thienyl)alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



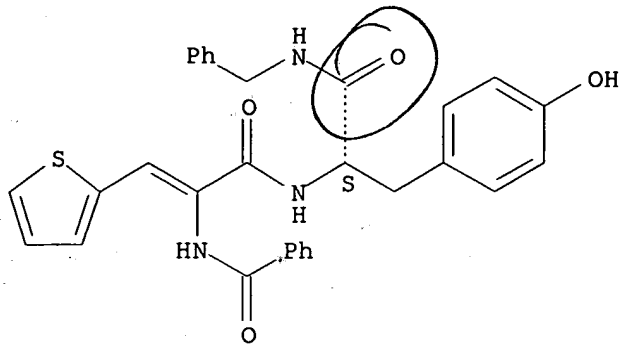
L27 ANSWER 68 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1979:474907 CAPLUS
DN 91:74907
TI Dehydrooligopeptides
IN Etschenberg, Eugen; Opitz, Wolfgang; Raddatz, Siegfried
PA Troponwerke G.m.b.H. und Co. K.-G., Fed. Rep. Ger.
SO Ger. Offen., 75 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2745584	A1	19790419	DE 1977-2745584	19771011
	NO 7704303	A	19780629	NO 1977-4303	19771214
	GB 1568137	A	19800529	GB 1977-53180	19771221
	AU 7731913	A1	19790628	AU 1977-31913	19771222
	AU 509040	B2	19800417		
	FI 7703922	A	19780629	FI 1977-3922	19771223
	SE 7714782	A	19780629	SE 1977-14782	19771227
	DK 7705815	A	19780629	DK 1977-5815	19771227
	NL 7714440	A	19780630	NL 1977-14440	19771227
	FR 2376128	A1	19780728	FR 1977-39354	19771227
	FR 2376128	B1	19800613		
	AT 7709326	A	19800515	AT 1977-9326	19771227
	AT 360185	B	19801229		
	JP 53082721	A2	19780721	JP 1977-157508	19771228
	ES 465518	A1	19790501	ES 1977-465518	19771228
	US 4276288	A	19810630	US 1979-82451	19791009
PRAI	DE 1976-2659114		19761228		
	DE 1977-2745584		19771011		
	US 1977-863208		19771222		

AB RCO-NHC(:CR1R2)CO-[NHC(:CR3R4)CO]m-[NR5CR6R7CO]n-R8 [I; R = alkyl, alkenyl, aryl, heterocyclic, aralkyl, aralkenyl, carbamoyl; R1 = H, alkyl; R2 = heterocyclic, aryl, aralkenyl, aralkyl, Et, cycloalkyl; R1R2=cyclopentylidene, cyclohexylidene, cyclopentenylidene, cyclohexenylidene; R3 = H, C1-2-alkyl; R4 = substituted Ph, aralkenyl, heterocyclic; R5 = H, alkyl; R6 = substituted CH2Ph, CH2OH, CH2CH2SMe, CH2CH2CONH2, CH2CH2CO2H; R7 = H; R5R6 = C2-4-alkylene; R6R7 = C4-5-alkylene; R8 = OH, NH2, NHR9, OR9 (R9 = alkyl, aryl, aralkyl), 5-or 6-membered N-contg. heterocyclic ring, alkylthio, NHNH2; m and n = 0, 1], useful as tumor- or tissue-dissolving agents with low toxicity, were prepd. by either treating oxazolone II with HNR5CR6R7COR8 or by hydrolyzing oxazolone III. Thus, oxazolone IV was treated with D-proline to give 55% AcNHC(:CHPh)CO-D-Pro-OH. Ninety other examples of I are given.

IT **68763-36-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 68763-36-0 CAPLUS
CN L-Tyrosinamide, N-benzoyl-2,3-didehydro-3-(2-thienyl)alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.


Ph
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OH
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S
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HN
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L27 ANSWER 69 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1979:104359 CAPLUS
DN 90:104359
TI Tumor- and tissue-dissolving pharmaceutical
IN Etschenberg, Eugen; Opitz, Wolfgang; Raddatz, Siegfried
PA Troponwerke G.m.b.H. und Co. K.-G., Fed. Rep. Ger.
SO Ger. Offen., 59 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 3

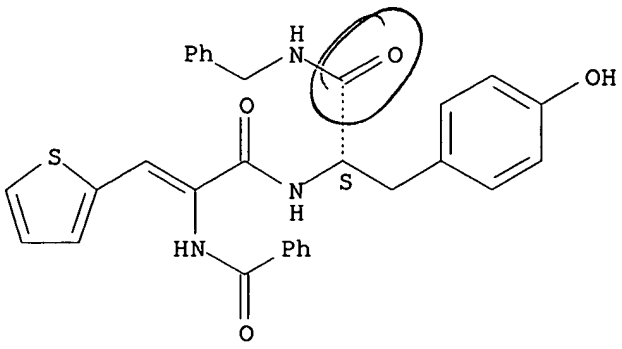
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2659154	A1	19780706	DE 1976-2659154	19761228
	AU 514183	B2	19810129	AU 1977-30457	19771108
	GB 1570140	A	19800625	GB 1977-53179	19771221
	AU 7731912	A1	19790628	AU 1977-31912	19771222
	BE 862329	A1	19780627	BE 1977-183848	19771227
	FR 2375867	A1	19780728	FR 1977-39353	19771227
	FR 2375867	B1	19800613		
	JP 53086043	A2	19780729	JP 1977-157507	19771228
	US 4310517	A	19820112	US 1979-82450	19791009
PRAI	DE 1976-2659154		19761228		
	DE 1977-2745673		19771011		
	US 1977-862896		19771221		

AB Dehydropeptides R(NR1CHR2CO)mNR3C(:CR4R5)CO(NR6CHR7CO)n[NR8C(:CR9R10)CO]p(NR11CR12R13CO)qR14 [R = H, alkoxycarbonyl, aralkoxycarbonyl, H2NCO, alkanoyl, alkenoyl, aroyl, aralkanoyl, aralkenoyl, lower alkylsulfonyl, arylsulfonyl, heteroaryl; R1, R6, and R11 = H, lower alkyl; R2, R7, and R12 = H, straight or branched lower alkyl, aryl, aralkyl, aralkenyl, indolylmethyl, heterocyclylmethyl with 1-2 hetero atoms in a 4-7-membered ring; R1R2, R6R7, and R11R12 = (CH2)3, (CH2)4; R3, R4, R8, and R9 = H, lower alkyl; R5 and R10 = alkyl, aryl, aralkyl, aralkenyl, 5-7-membered heterocyclic ring with 1-2 hetero atoms; R4R5 and R9R12 = (CH2)r (r = 3-7); R13 = H; R12R13 = (CH2)s (s = 4-7); R14 = OH, lower alkoxy, lower alkenyloxy, NH2, alkylamino, dialkylamino, alkenylamino, dialkenylamino, arylamino, aralkylamino, diaralkylamino, 4-7-membered N-contg. heterocyclic ring with 1-2 hetero atoms, NHR15 (R15 = 3-7-membered alicyclic ring; m, n, p, and q = 0, 1] and their pharmaceutically acceptable salts were prepd. as tumor- and tissue-dissolving pharmaceuticals. Thus, oxazolone I was sapond. with 2N NaOH to give 84.5% dehydrodipeptide DL-AcNHC(:CHPh)CONHCH(CH2C6H4Cl-3)CO2H. Oxazolone II was treated with proline in acetone to give 59% AcNHC(:CHPh)CO-Pro-OH. Approx. 78 dehydro derivs. were prepd.

IT **68763-36-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 68763-36-0 CAPLUS
CN L-Tyrosinamide, N-benzoyl-2,3-didehydro-3-(2-thienyl)alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.


Ph
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H
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HN
Ph
O

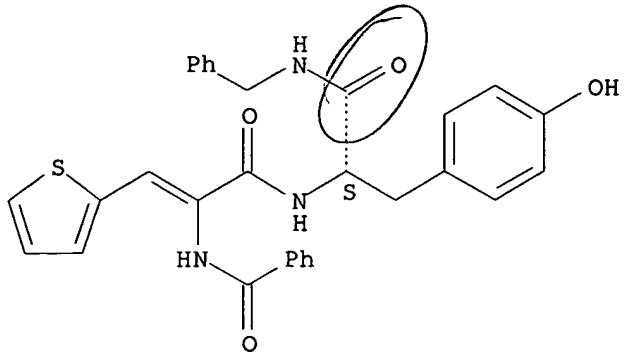
L27 ANSWER 70 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1979:55277 CAPLUS
DN 90:55277
TI Dehydrooligopeptides
IN Etschenberg, Eugen; Opitz, Wolfgang; Raddatz, Siegfried
PA Troponwerke G.m.b.H. und Co. K.-G., Fed. Rep. Ger.
SO Ger. Offen., 60 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2659114	A1	19780706	DE 1976-2659114	19761228
	NO 7704303	A	19780629	NO 1977-4303	19771214
	GB 1568137	A	19800529	GB 1977-53180	19771221
	AU 7731913	A1	19790628	AU 1977-31913	19771222
	AU 509040	B2	19800417		
	FI 7703922	A	19780629	FI 1977-3922	19771223
	BE 862330	A1	19780627	BE 1977-183849	19771227
	SE 7714782	A	19780629	SE 1977-14782	19771227
	DK 7705815	A	19780629	DK 1977-5815	19771227
	NL 7714440	A	19780630	NL 1977-14440	19771227
	FR 2376128	A1	19780728	FR 1977-39354	19771227
	FR 2376128	B1	19800613		
	AT 7709326	A	19800515	AT 1977-9326	19771227
	AT 360185	B	19801229		
	JP 53082721	A2	19780721	JP 1977-157508	19771228
	ES 465518	A1	19790501	ES 1977-465518	19771228
	US 4276288	A	19810630	US 1979-82451	19791009
PRAI	DE 1976-2659114		19761228		
	DE 1977-2745584		19771011		
	US 1977-863208		19771222		

AB Dehydropeptides RCONHC(:CR1R2)CO[NHC(:R3R4)CO]m[NR5CR6R7CO]nR8 [R = alkyl, aryl, heterocyclic, aralkyl, aralkenyl; R1 = H, lower alkyl, R2 = heterocyclic, aryl, aralkenyl, aralkyl, Et, cycloalkyl; CR1R2 = cyclopentylidene, cyclohexylidene, cyclopentenylidene, cyclohexenylidene; R3 = H, C1-2 alkyl; R4 = substituted Ph, aralkenyl, heterocyclic; R5 = H, alkyl; R6 = substituted CH2Ph, CH2OH, CH2CH2SMe, CH2CH2CONH2, CH2CH2CO2Et; R5R6 = (CH2)3, (CH2)4; R7 = H, R6R7 = (CH2)4, (CH2)5; R8 = NHR9 (R9 = H, alkyl, aryl, arakyl), 5-7-membered N-contg. heterocyclic ring, OR10 (R10 = H, aralkyl, alkyl, aryl), m and n = 0, 1] and physiol. acceptable salts were prepd. as tumor- and tissue-dissolving agents. Thus, oxazolone I was treated with D-proline to give 55% AcNHC(:CHPh)CO-D-Pro-OH. Oxazolone II was sapond. with N NaOH in Me2CO to give 56.4% AcNHC(:CHPh)CONHC(:CHC6H4NO2-4)CO2H. Approx. 49 dehydropeptides were prepd.

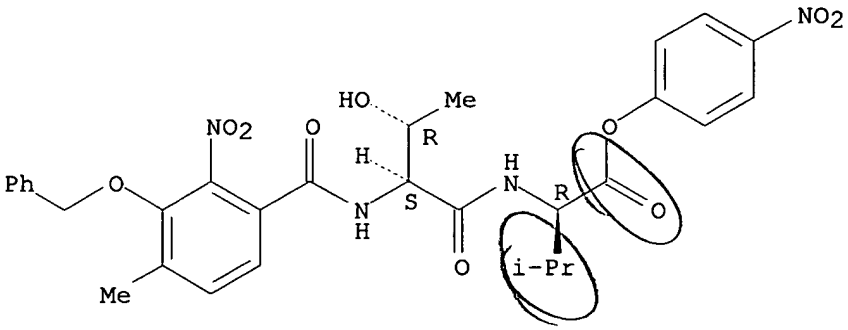
IT **68763-36-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 68763-36-0 CAPLUS
CN L-Tyrosinamide, N-benzoyl-2,3-didehydro-3-(2-thienyl)alanyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.


Ph
H
N
O
OH
O
S
N
H
S
HN
Ph
O

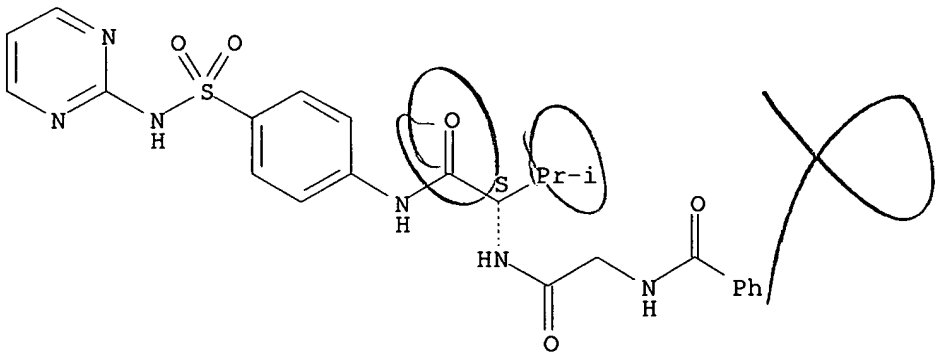
L27 ANSWER 71 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1978:499896 CAPLUS
DN 89:99896
TI Synthesis and evaluation of bis-dipeptide and bis-tripeptide analogs of actinomycin D
AU Chowdhury, A. K. Azad; Brown, Jeffrey R.; Longmore, Robert B.
CS Dep. Pharm., Univ. Manchester, Manchester, UK
SO Journal of Medicinal Chemistry (1978), 21(7), 607-12
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
AB Six bis-dipeptide analogs of actinomycin D (I) [50-76-0] contg. 2 threonyl-D-valine side chains and 2 bis-tripeptide analogs contg. an addn. proline or oxoproline residue were synthesized. None of the compds. bound to DNA in a manner similar to I. None of the analogs tested had antitumor activity. II [66702-04-3] exhibited the most potent antibacterial activity, a measure of cytotoxicity, against Bacillus subtilis which was approx. 10% of the potency of I.
IT **66682-59-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and hydrolysis of)
RN 66682-59-5 CAPLUS
CN D-Valine, N-[N-[4-methyl-2-nitro-3-(phenylmethoxy)benzoyl]-L-threonyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



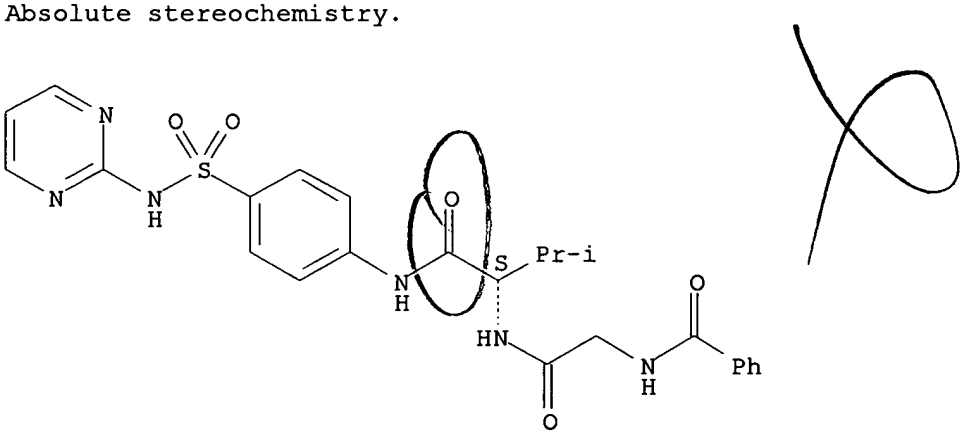
L27 ANSWER 72 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1977:439805 CAPLUS
DN 87:39805
TI Synthesis of some N4-(amino acid or dipeptide)-sulfanilamide derivatives
AU El-Naggar, A. M.; Zaher, M. R.
CS Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SO Roczniki Chemii (1976), 50(12), 2187-91
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA English
AB 4-RNHC6H4SO2NHR1 [I; R = Bz-Gly, R1 = H, R2, R3, C(:NH)NH2; R = Tos-.beta.-Ala, R1 = R2, C(:NH)NH2; where Tos = 4-MeC6H4SO2] were prepd. by condensing R-NHNH, with the appropriate 4-H2NC6H4SO2NHR1 (II) by azide couplings. I (R = phthaloylglycyl, phthaloyl-.beta.-alanyl, R1 = H, R3; R = Tos-.beta.-Ala, Tos-Ala, R1 = R3) were prepd. by acylating the appropriate II with the appropriate R-Cl. Bz-Gly-NHNH2 was coupled to H-X-OMe (X = Ala, Val) to give Bz-Gly-X-OMe which were treated with NH2NH2 to give Bz-Gly-X-NHNH2 (III). Bz-Gly-X-NHC6H4SO2NHR1 (IV; X = Ala, R1 = R2, R3; X = Val, R1 = R3) were prepd. by coupling III to the appropriate II. I (X = Tos-.beta.-Ala, Tos-Ala; R1 = R3) possess antibacterial against Bacillus subtilis and Escherichia coli, but they were inactive against Micrococcus pyogenes and several other bacteria. IV (X = Ala, R1 = R2) was active against B. subtilis and inactive against all other microorganisms tested.
IT **63203-27-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 63203-27-0 CAPLUS
CN L-Valinamide, (N-benzoylglycyl)-N-[4-[(2-pyrimidinylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



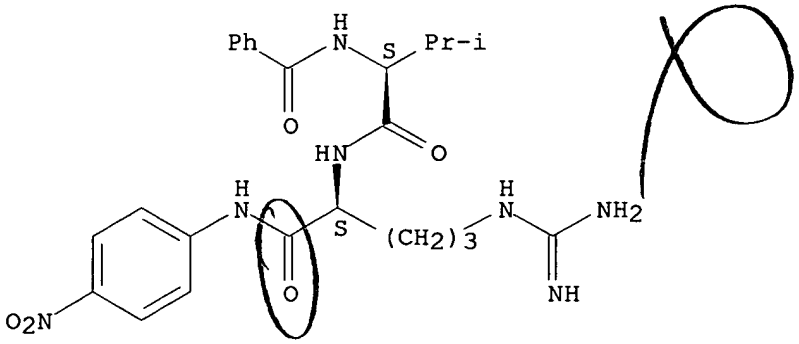
L27 ANSWER 73 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1977:433009 CAPLUS
DN 87:33009
TI Metal complexes and biological activities of some peptides containing glycine, alanine, and hippuric acid
AU El-Naggar, A. M.; Shehata, Y. A.; Zaher, M. R.
CS Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SO Roczniki Chemii (1977), 51(2), 233-7
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA English
AB Spectrophotometric studies were carried out on the formation of Cu, Fe, and Ni complexes with di- and tripeptides contg. glycine, alanine, and hippuric acid. Replacement of the end amino acid in the peptide by 2-aminopyridine, sulfadiazine, sulfathiazole, sulfanilamide, sulfaguanidine, urea, or .beta.-alanine gave compds. which did not form the normal complexes with Cu2+, Fe3+, and Ni2+ ions. The hydrazides of the peptides participated in the usual way in the formation of complexes. Some of the obtained complexes exhibited distinct antibacterial activity.
IT **63203-27-0DP**, copper complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 63203-27-0 CAPLUS
CN L-Valinamide, (N-benzoylglycyl)-N-[4-[(2-pyrimidinylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 74 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1973:94260 CAPLUS
DN 78:94260
TI Substrates for determination of trypsin, thrombin, and thrombin-like enzymes
AU Svendsen, L.; Blomback, B.; Blomback, M.; Olsson, P. I.
CS Dep. Blood Coagulation Res., Karolinska Inst., Stockholm, Swed.
SO Folia Haematologica (Leipzig) (1972), 98(4), 446-54
CODEN: FOHEAW; ISSN: 0323-4347
DT Journal
LA English
AB Various p-nitroaniline derivs. of peptides such as H-Phe-Val-Arg-OH were susceptible to the action of trypsin, thrombin, and reptilase.
IT **38789-82-1**
RL: BIOL (Biological study)
(as proteinase detn. substrate)
RN 38789-82-1 CAPLUS
CN L-Argininamide, N-benzoyl-L-valyl-N-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

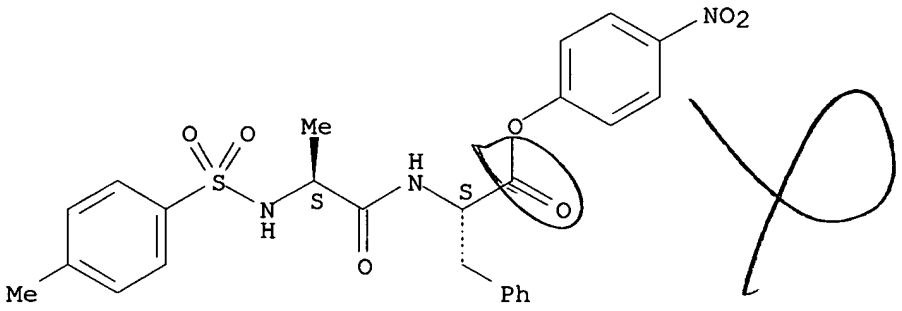
Absolute stereochemistry.



● HCl

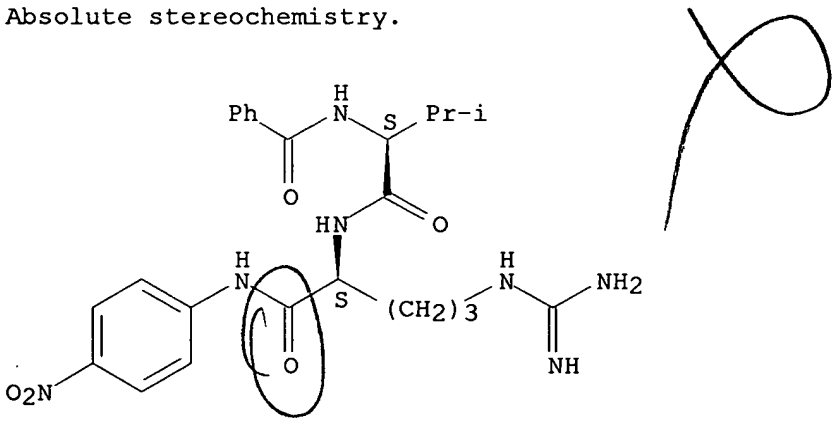
L27 ANSWER 75 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1973:16465 CAPLUS
DN 78:16465
TI Cyclization of activated p-toluenesulfonyl peptides
AU Lucente, Gino; Frattesi, Patrizia
CS Ist. Chim. Farm., Univ. Studi, Rome, Italy
SO Tetrahedron Letters (1972), (42), 4283-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
AB Tos-L-Ala-L-Phe-ONP, Tos-L-Ala-L-Phe-L-Pro-ONP and Tos-L-Ala-D-Phe-L-Pro-ONP (Tos = p-tolylsulfonyl; ONP = p-nitrophenyl ester) in mild aq. alk. gave 3(S)-benzyl-6(S)-methyl-1-(p-tolylsulfonyl)-2,5-piperazinedione, [N-(p-tolylsulfonyl)-L-alanyl-L-phenylalanyl-D-proline anhydride, and [N-(p-tolylsulfonyl)-L-alanyl]-D-phenylalanyl-L-proline anhydride, resp.
IT **40056-01-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 40056-01-7 CAPLUS
CN L-Phenylalanine, N-[N-[(4-methylphenyl)sulfonyl]-L-alanyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



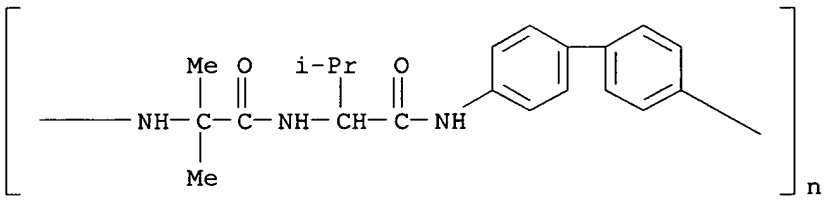
L27 ANSWER 76 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1972:536733 CAPLUS
DN 77:136733
TI Synthetic chromogenic substrates for determination of trypsin, thrombin, and thrombinlike enzymes
AU Svendsen, Lars; Blomback, Birger; Blomback, Margareta; Olsson, Per I.
CS Dep. Blood Coagulation Res., Karolinska Inst., Stockholm, Swed.
SO Thrombosis Research (1972), 1(3), 267-78
CODEN: THBRAA; ISSN: 0049-3848
DT Journal
LA English
AB These new synthetic substrates consist of arginine p-nitroanilides in which the NH2 group of arginine is acylated with hydrophobic amino acids or peptides. Benzoylation of the free NH2-terminal group enhances the susceptibility of the peptide substrates. One of the most reactive substrates is N.alpha.-benzoyl - phenylalanyl - valyl - arginine p-nitroanilide (Bz-Phe-Val-Arg-pNA). Some kinetic parameters for these substrates with trypsin, thrombin, and reptilase were studied. Trypsin has a much higher affinity for Bz-Phe-Val-Arg-pNA than for benzoyl-DL-arginine p-nitroanilide (BAPNA). The former substrate has a high susceptibility toward thrombin and reptilase. The narrow substrate specificity of thrombin as compared with trypsin is reflected by the fact that Bz-L-Phe-L-Val-L-Arg-pNA is rapidly hydrolyzed by thrombin while the hydrolysis rate of Bz-D-Phe-L-Val-L-Arg-pNA is very slow. With trypsin, the action on the D-isomer is only slightly reduced. These synthetic peptide substrates are useful for spectrophotometric detn. of enzymes of the trypsin type, and they can also be used in biol. fluids. They allow small amts. of trypsin, thrombin, and reptilase to be detd.
IT **38789-82-1**
RL: BIOL (Biological study)
(in thrombin and trypsin detn.)
RN 38789-82-1 CAPLUS
CN L-Argininamide, N-benzoyl-L-valyl-N-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

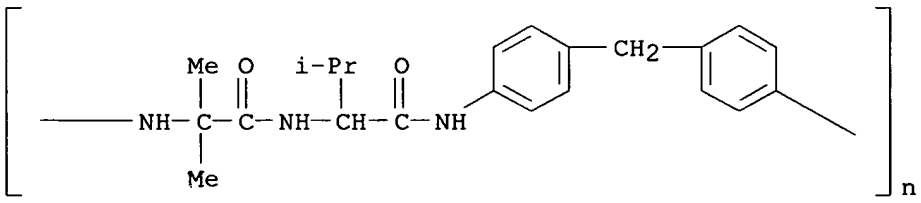


● HCl

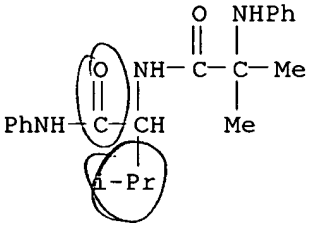
L27 ANSWER 77 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1968:105573 CAPLUS
DN 68:105573
TI Synthesis of poly(amideamines) from 5-oxazolones
AU Iwakura, Yoshio; Toda, Fujio; Torii, Yoshinori; Murata, Katsuaki
CS Univ. Tokyo, Tokyo, Japan
SO Journal of Polymer Science, Part A: General Papers (1968), 6(4), 785-91
CODEN: JPYAAK; ISSN: 0449-2951
DT Journal
LA English
AB Poly(amide amines) with a sequence of two amide and one amine linkages in a main chain were synthesized from the polyaddn. of 2-isopropylidene-4-alkyl-3-oxazolin-5-ones and primary diamines. The polyaddn. reaction proceeded through 1,4-conjugate addn. of an amine group to 3-oxazolin-5-one and subsequent ring opening of the intermediate addn. product with another amine. Although aliphatic diamines gave oily polymers, xylylenediamines afforded amorphous solid polymers. The reduced viscosities and polymer melt temp. of the polymers were 0.05-0.12 and 90-130.degree., resp. 16 references.
IT **32037-36-8P 32037-37-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 32037-36-8 CAPLUS
CN Poly(iminocarbonylisobutylideneiminocarbonylisopropylideneimino-4,4'-biphenylylene) (8CI) (CA INDEX NAME)



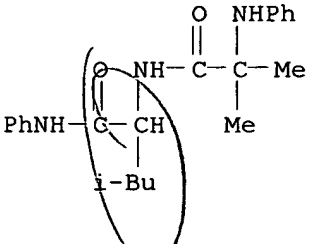
RN 32037-37-9 CAPLUS
CN Poly(iminocarbonylisobutylideneiminocarbonylisopropylideneimino-p-phenylenemethylene-p-phenylene) (8CI) (CA INDEX NAME)



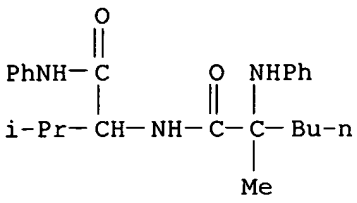
L27 ANSWER 78 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1968:39524 CAPLUS
DN 68:39524
TI Reaction of alkylidenepseudoxazolones with amines
AU Iwakura, Yoshio; Toda, Fujio; Torii, Yoshinori; Tomioka, Kozaburo
CS Univ. Tokyo, Tokyo, Japan
SO Tetrahedron (1967), 24(2), 575-83
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
AB New 2-alkylidenepseudoxazolones (I) reacted with primary amines to give 1:2-addn. products while I in the reaction with secondary amines gave mixts. of 1:1- and 1:2-adducts. A relation of the structures of pseudoxazolones and amines to the products was discussed. 25 references.
IT **14839-74-8P 14839-90-8P 17548-03-7P**
17548-16-2P 17548-17-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 14839-74-8 CAPLUS
CN Butyranilide, 2-(2-anilino-2-methylpropionamido)-3-methyl- (8CI) (CA INDEX NAME)



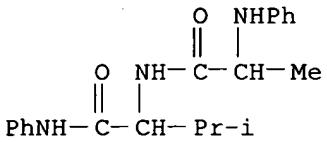
RN 14839-90-8 CAPLUS
CN Valeranilide, 2-(2-anilino-2-methylpropionamido)-4-methyl- (8CI) (CA INDEX NAME)



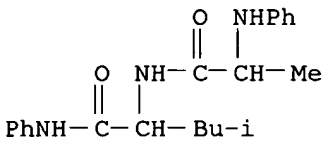
RN 17548-03-7 CAPLUS
CN Butyranilide, 2-(2-anilino-2-methylhexanamido)-3-methyl- (8CI) (CA INDEX NAME)



RN 17548-16-2 CAPLUS
CN Butyranilide, 2-(2-anilinopropionamido)-3-methyl- (8CI) (CA INDEX NAME)

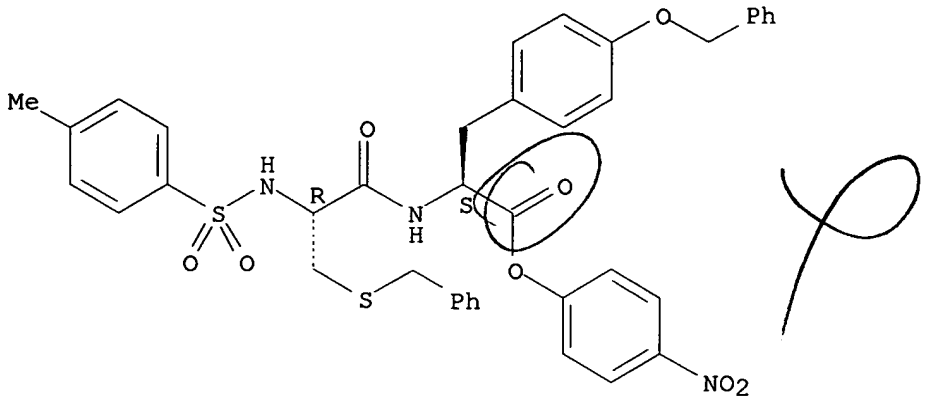


RN 17548-17-3 CAPLUS
CN Valeranilide, 2-(2-anilinopropionamido)-4-methyl- (8CI) (CA INDEX NAME)



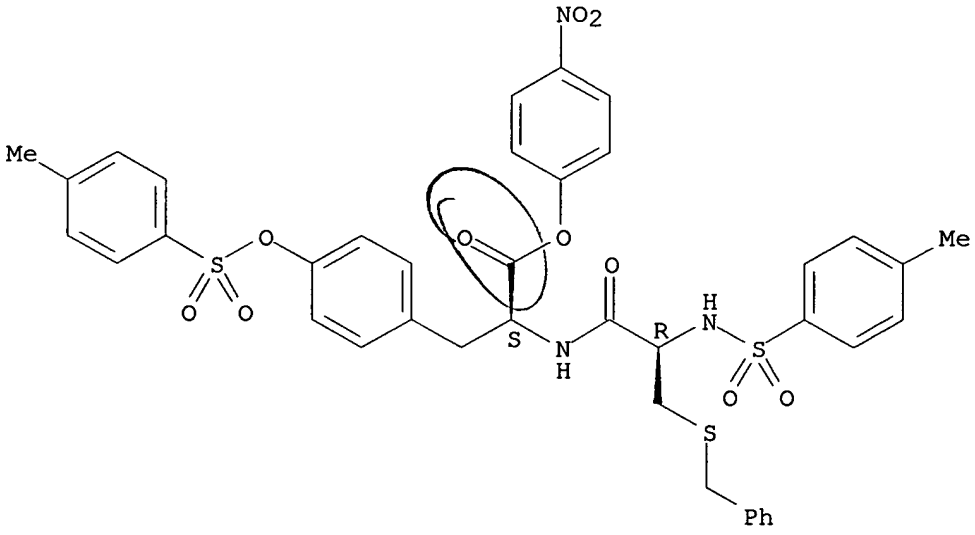
L27 ANSWER 79 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1967:444069 CAPLUS
DN 67:44069
TI Amino acids and peptides. LXXII. Synthesis of 2-phenylalanine-[U-14C] 8-lysine vasopressin
AU Thomas, Patrick Jonathan; Havranek, M.; Rudinger, Josef
CS Ceskoslov. Akad. Ved, Prague, Czech.
SO Collection of Czechoslovak Chemical Communications (1967), 32(5), 1767-75
CODEN: CCCCAK; ISSN: 0010-0765
DT Journal
LA English
AB CA 66: 86017h. In this abstr., Z = benzyloxycarbonyl, BZL = PhCH2, TOS = tosyl, NPS = o-nitrophenylsulfenyl, Np = p-C6H4NO2; all amino acids are of the L configuration. Z-Phe (19.0 mg.), obtained in 88.5% yield from the labeled amino acid, was shaken in 0.29 ml. MeCN and 24.62 mg. N-methylpiperidine with 16.8 mg. 2-ethyl-5-phenylisoxazolium 3'-sulfonate until dissolved, 61.9 mg. Gln-Asn-Cys(BZL)-Pro-Lys(TOS)-Gly-NH2 in 0.55 ml. HCONMe2 added and the mixt. kept 24 hrs. to give 64.7 mg. Z-Phe-Gln-Asn-Cys(BZL)-Pro-Lys(TOS)-Gly-NH2 (I), m. 182-8.degree.. Treating I with 0.7 ml. 35% HBr soln. in AcOH gave 71% Phe-Gln-Asn-Cys(BZL)-Pro-Lys(TOS)-Gly-NH2 (II), m. 130-5.degree.. II (41.1 mg.) was coupled as usual with TOS-Cys(BZL)-Tyr-N3 (from 215.5 mg. hydrazile) to give 39 mg. TOS-Cys(BZL)-Tyr-Phe-Gln-Asn-Cys(BZL)-Pro-Lys(TOS)-Gly-NH2, m. 187-95.degree., which was treated with Na in liquid NH3 to give the title compd. (III) in 8.5% overall yield (specific radioactivity 5.8 c./mg., radioactivity: pressor activity 2.60 m.mu.c./I.U.). By an alternative route, NPS-Tyr(BZL), m. 136-9.degree., gave with p-O2NC6H4OH and dicyclohexylcarbodiimide in AcOEt 76% NPS-Tyr(BZL)-ONp, m. 148-54.degree., which was converted with 7M HCl-Et2O to 90% Tyr(TOS)-ONp.HCl, m. 155-65.degree., and this, in turn, shaken with TOS-Cys(BZL)-Cl to yield 79% TOS-Cys(BZL)-Tyr(BZL)-ONp (IV), m. 166-7.degree.. IV (45 mg.) was coupled with 31.3 mg. II to give 64% TOS-Cys(BZL)-Tyr(BZL)-Phe-Gln-Asn-Cys(BZL)-Pro-Lys(TOS)-Gly-NH2, m. 190-200.degree., [.alpha.]25D -26.2.degree. (c 0.5, HCONMe2), yielding as above III in 13.7% overall yield. As a variation of the 2nd method, NPS-Tyr(TOS), m. 144-8.degree., was converted to 58% NPS-Tyr(TOS)-ONp, m. 119-21.degree., which treated with 6.85M HCl-Et2O and the HCl salt of Tyr(TOS)-ONp, m. 175-80.degree., acylated as above to give 56% TOS-Cys(BZL)-Tyr(TOS)-ONp, m. 128-31.degree., or coupled with II to yield 84% TOS-Cys(BZL)-Tyr(TOS)-Phe-Gln-Asn-Cys(BZL)-Pro-Lys(TOS)-Gly-NH2, m. 180-92.degree., [.alpha.]D -29.3.degree. (c 0.5, HCONMe2).
IT **15396-65-3P 15396-86-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 15396-65-3 CAPLUS
CN Alanine, 3-[p-(benzyloxy)phenyl]-N-[3-(benzylthio)-N-(p-tolylsulfonyl)-L-alanyl]-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



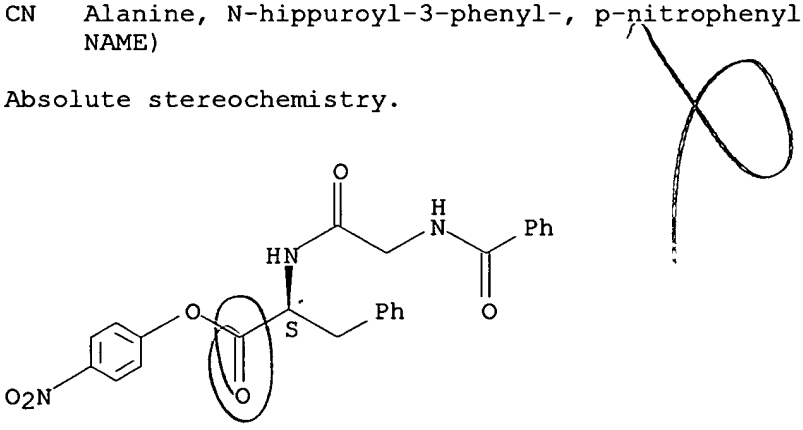
RN 15396-86-8 CAPLUS
CN Tyrosine, N-[3-(benzylthio)-N-(p-tolylsulfonyl)-L-alanyl]-, p-nitrophenyl ester, p-toluenesulfonate (ester), L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



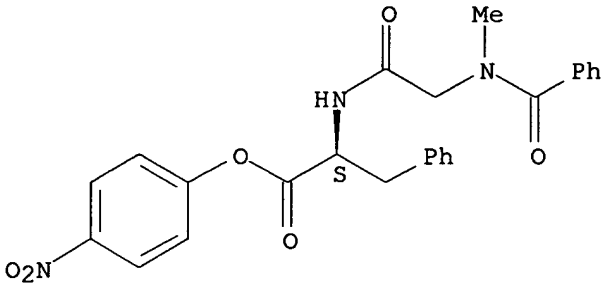
L27 ANSWER 80 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1967:105183 CAPLUS
DN 66:105183
TI Amino acids and peptides. XXV. The mechanism of the base-catalyzed racemization of the p-nitrophenyl esters of acylpeptides
AU Antonovics, Ieva; Young, Geoffrey Tyndale
CS Oxford Univ., Oxford, UK
SO Journal of the Chemical Society [Section] C: Organic (1967), (7), 595-601
CODEN: JSOOAX; ISSN: 0022-4952
DT Journal
LA English
AB cf. CA 64, 5200f. The p-nitrophenyl esters of benzoyl- and benzyloxycarbonyl glycyl-L-phenylalanine (I) are racemized by Et3N in CH2Cl2 much more rapidly than are the analogous esters of benzyloxycarbonyl- and phthaloyl-L-phenylalanine. The acyldipeptide esters react reversibly with Et3N to give the corresponding oxazolone, the equil. being greatly in favor of the ester. The racemization of benzoylglycyl-L-phenylalanine p-nitrophenyl ester by Et3N is suppressed by the addn. of a large excess of the oxazolone derived from benzyloxycarbonylglycylphenylalanine, which reacts immediately with the p-nitro-phenoxide anion and so prevents the back-reaction by which racemic ester is formed. This expt. distinguishes clearly between the direct exchange mechanism of racemization and that through the oxazolone. Such racemization proceeds through the intermediate formation, racemization, and coupling of the corresponding oxazolone. Evidence is also given that the conversion of I into its p-nitrophenyl ester by means of diphenylketene is accompanied by racemization. 23 references.
IT **2900-37-0P 13836-51-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and racemization of)
RN 2900-37-0 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



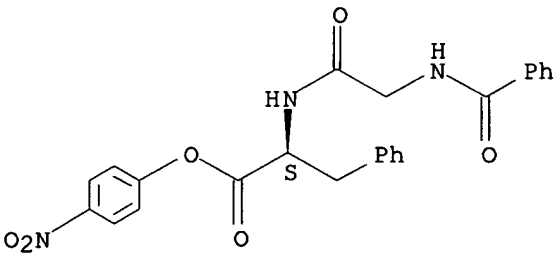
RN 13836-51-6 CAPLUS
CN Alanine, N-(.beta.-methylhippuroyl)-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

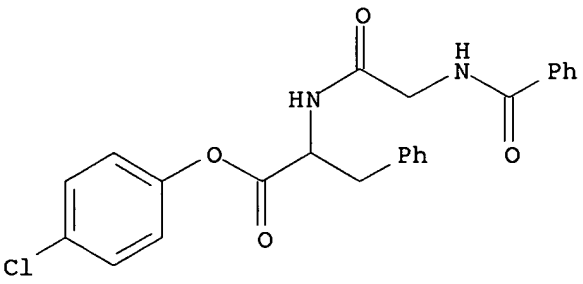


IT **2900-37-0P 13716-78-4P 13716-80-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 2900-37-0 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

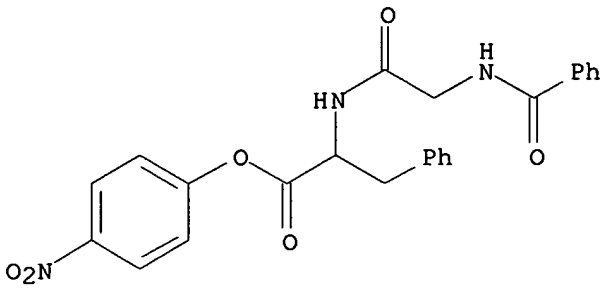
Absolute stereochemistry.



RN 13716-78-4 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-chlorophenyl ester, DL- (8CI) (CA INDEX NAME)



RN 13716-80-8 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, DL- (8CI) (CA INDEX NAME)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H
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HN
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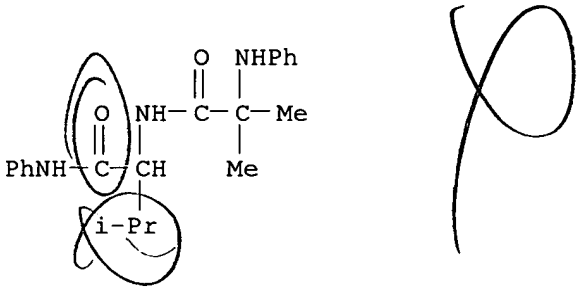
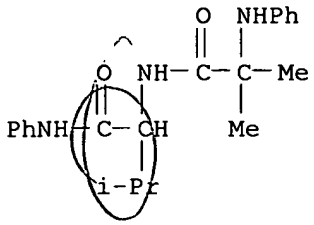
L27 ANSWER 81 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1967:65906 CAPLUS
DN 66:65906
TI A novel synthesis of poly(amide amines) from 5-oxazolones
AU Iwakura, Yoshio; Toda, Fujio; Torii, Yoshinori
CS Univ. Tokyo, Tokyo, Japan
SO Journal of Polymer Science, Polymer Letters Edition (1967), 5(1), 17-21
CODEN: JPYBAN; ISSN: 0360-6384
DT Journal
LA English
AB 2-Isopropylidene-4-isopropyl-3-oxazolin-5-one (I), prepd. by the ring closure of the corresponding N-methacryloyl-.alpha.-amino acid by Ac2O in pyridine, reacts with 2 moles of aniline, giving .alpha.-(.alpha.'-anilinoisobutyramido)isovaleric acid anilide. The benzylamine-I adduct is similarly prepd. I, 2-isopropylidene-4-methyl-3-oxazolin-5-one (II), and 2-isopropylidene-4-isobutyl-3-oxazolin-5-one (III) were copolymd. with m-xylylenediamine in dioxane at 60.degree. giving poly(amide amines) (IV). NH2(CH2)nNH2, where n = 2, 3, 4, or 6, gave low melting polymeric oils with I, II, or III. p-Phenylenediamine polymd. only very slowly.
IT **14839-74-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 14839-74-8 CAPLUS
CN Butyranilide, 2-(2-anilino-2-methylpropionamido)-3-methyl- (8CI) (CA INDEX NAME)

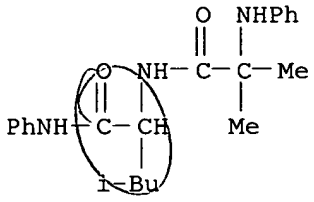


L27 ANSWER 82 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1967:64785 CAPLUS
DN 66:64785
TI Reaction of alkylidenepseudoxazolones with amines
AU Iwakura, Yoshio; Toda, Fujio; Torii, Yoshinori; Tomioka, Kozaburo
CS Univ. Tokyo, Tokyo, Japan
SO Tetrahedron Letters (1966), (45), 5461-6
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
AB Treatment of 2-isopropylidene-4-R-substituted 3-oxazolin-5-ones (I) (R = Me) (Ia), I (R = Me2CH) (II), I (R = Me2CHCH2) with 2 moles PhNH2 at 60.degree. 12-24 hrs. reacted quant. to give, resp., the anilides PhNHCMe2CONHCHRCONHPh (III) (R, m.p., and % yield given): Me (IV), 140-2.degree., 43; Me2CH (V), 174-6.degree., 99; Me2CHCH2 (VI), 171-3.degree., 63. The N.M.R. spectrum of IV showed peaks at .delta. 1.60 s, 1.44 (J 6.6) in C5H5N. IV was partially hydrolyzed in 2 hrs. at 100-120.degree. with concd. HCl to give 63% PhNHCMe2CONHCHMeCO2H, m. 187-8.degree., and completely hydrolyzed at 160.degree. with concd. HCl for 16 hrs. to 59% PhNHCMe2CO2H, m. 180-2.degree., and MeCH(NH2)CO2H: N-benzoyl deriv., m. 159-61.degree.. Complete hydrolysis of V and VI similarly gave PhNHCMe2CO2H and valine and leucine, resp. Addn. to PhLi to dimethylfulvene gave VII and various M.O. calcns. on fulvene and its derivs. have suggested an appreciable drift of electrons from the exo double bond into the ring (Smith and Shoulders, CA 61, 6897b). The exo double bond of I would become a reaction center of nucleophilic reagents by a similar electron drift. Accordingly a 1,4-conjugate addn. of PhNH2 to the Me2C:C-N-C-R chain followed by a ring opening was postulated as a probable reaction mechanism. II treated with the primary amines PhCH2NH2, PhCH2CH2, and cyclohexylamine gave, resp., 1:2 adducts, m. 89-92.degree., 120-2.degree., and 127-9.degree. in 91, 20, and 33% yields. With piperidine II yielded 73% 1:1 adduct (VIII), Me2CHCONHC(:CMe2)CONC5H10, m. 129-31.degree., identical with a compd. obtained from 2-isopropyl-4-isopropylidene-2-oxazolin-5-one (IX), and piperidine. IX was prepd. in 11% yield from Me2CHCH2NHCH2CO2H by the method of Erlenmeyer (Ramage and Simonsen, CA 29, 65919). VIII was accompanied by a small amt. (17%) of 1:2 adduct, m. 95-6.degree., with a structure analogous to III. II and morpholine gave 77% 1:2 adduct, m. 119-22.degree., but with PhCH2NHMe and pyrrolidine only the 1:1 adducts, m. 117-18.degree. and 154-6.degree. were obtained in 22 and 68% yields, resp. A tautomeric equil. is readily established between the pseudooxazolones I and the corresponding unsatd. 5-oxazolone. However, the products formed by the methods of Iwakura, et al. and Erlenmeyer were II and IX, resp., and were not interconvertible in boiling C5H5N. Treatment of fractionally distd. pure 2-ethylidene-4-alkyl-3-oxoazolin-5-ones (alkyl = R = Me2, Me2CH, Me2CHCH2) with PhNH2 gave a mixt. of 1:1 and 1:2 adducts (R, m.p. 1:1 adduct, and m.p. 1:2 adduct given): Me, 172-5.degree., 147-51.degree.; Me2CH, -, 150-1.degree.; Me2CHCH2, 200.degree., 145.degree.. IX gave 43% 1:1 adduct, m. 242-3.degree., and 2-ethyl-4-isopropylidene-2-oxazoline-5-one similarly gave a 1:1 adduct, m. 205-7.degree.. Ia and m-H2NCH2C6H4CH2NH2 gave a new type of polymeric adduct, -CMe2CONHCHMeCONHCH2C6H4CH2NH-, .eta.sp/C, c 0.5, 0.18, in HCONMe2. PhSH also gave with II 17% 1:2 adduct, m. 120-2.degree..
IT **14839-74-8P 14839-90-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 14839-74-8 CAPLUS
CN Butyranilide, 2-(2-anilino-2-methylpropionamido)-3-methyl- (8CI) (CA

INDEX NAME)

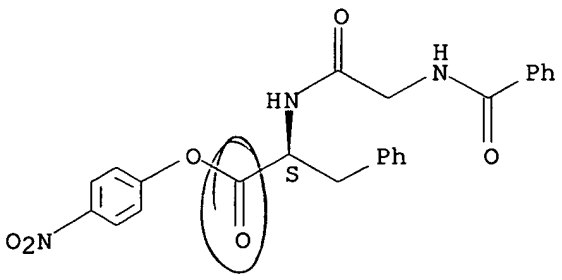


RN 14839-90-8 CAPLUS
CN Valeranilide, 2-(2-anilino-2-methylpropionamido)-4-methyl- (8CI) (CA INDEX NAME)



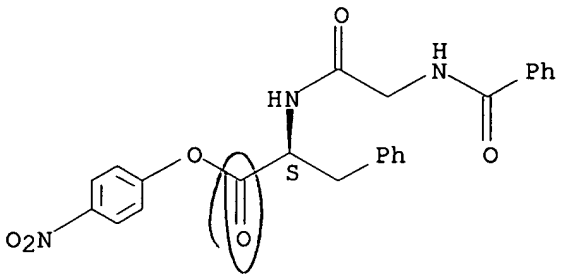
L27 ANSWER 83 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1965:489240 CAPLUS
DN 63:89240
OREF 63:16450d-f
TI Contribution to the discussion on racemization
AU Young, G. T.; Antonovics, I.
SO Acta Chimica Academiae Scientiarum Hungaricae (1965), 44(1-2), 43-4
CODEN: ACASA2; ISSN: 0001-5407
DT Journal
LA English
AB cf. preceding abstr. When benzoylglycyl-L-phenylalanine p-nitrophenyl ester in tetrahydrofuran was treated with one equiv. of Et3N the optical rotation fell very much more rapidly than when the benzyloxycarbonyl(CBZ)-L-phenylalanine ester was similarly treated, and when CH2Cl2 was used as solvent, benzoylglycyl-DL-phenylalanine p-nitrophenyl ester sepd. out within 1 hr. at room temp. However, the ir absorption of the soln. showed only a very small peak at 1830 cm.-1 (oxazolone C:O), and the same observation was made with the CBZ analog. Addn. of 1 equiv. each of Et3N and p-nitrophenol to the oxazolones very rapidly extinguished the 1830 cm.-1 peak. Equimolar amts. of CBZ-L-phenylalanine p-nitrophenyl ester and of the oxazolone derived from benzoylglycyl-L-phenylalanine in CH2Cl2 were treated with one equiv. of Et3N 1 hr. at room temp. The p-nitrophenyl ester was recovered. Chromatography showed the presence of the p-nitrophenyl esters of both the CBZ-and the benzoyl-dipeptide esters, and the latter ester was isolated (as racemate). This evidence is viewed as consistent with racemization proceeding through the oxazolone formed rapidly but being present in only small concn.
IT **2900-37-0**, Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L-
(coupling reactions of, racemization in relation to)
RN 2900-37-0 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L27 ANSWER 84 OF 84 CAPLUS COPYRIGHT 2003 ACS
AN 1965:480972 CAPLUS
DN 63:80972
OREF 63:14976g-h
TI The mechanism of racemization during the coupling of acyl peptides
AU Antonovics, I.; Young, G. T.
CS Univ. Oxford, UK
SO Chemical Communications (London) (1965), (17), 398-9
CODEN: CCOMA8; ISSN: 0009-241X
DT Journal
LA English
AB When a soln. of benzoyl-L-leucine p-nitrophenyl ester in dichloromethane was treated with one molar proportion of triethylamine, the optical rotation decreased by 50% in 50 min. at room temp. -far more rapidly than with phthaloyl-L-phenylalanine p-nitrophenyl ester (.apprx. 5% in the same time). It was concluded that the racemization followed chiefly, if not exclusively, through the oxazolone.
IT **2900-37-0**, Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (coupling and racemization of)
RN 2900-37-0 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



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L9               QUE L8 AND L6 NOT L7
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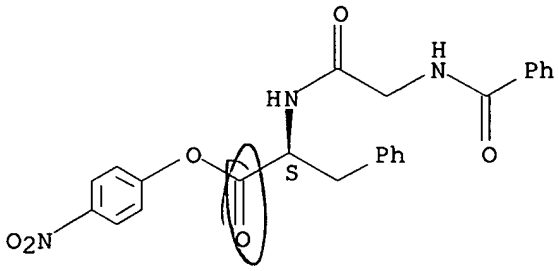
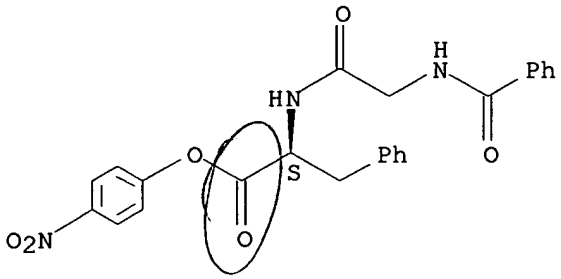
L28 ANSWER 1 OF 2 CAOLD COPYRIGHT 2003 ACS
AN CA63:16450d CAOLD
TI racemization
AU Young, Geoffrey T.; Antonovics, I.
IT **2900-37-0**
RN 2900-37-0 CAOLD
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 2 OF 2 CAOLD COPYRIGHT 2003 ACS
AN CA63:14976h CAOLD
TI synthesis of peptides related to eledoisin
AU Boissonnas, Roger A.; Sandrin, E.
IT **2900-37-0**
RN 2900-37-0 CAOLD
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



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